United States Department of the Interior
Geological Survey

The U. S. Geological Survey Instrument for Simultaneous Multi-element Atomic Absorption Spectrometry:

Description of the Hardware and of the System Control and Data Acquisition Software

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INTRODUCTION

Historically, atomic absorption spectrometry (AAS) was developed as an inherently single element technique. A single element technique is one that is capable of measuring a signal related to concentration for only one element at a time. Despite this limitation to the rate of measurements, conventional AAS has been a principal technique for geochemical analysis of samples in solution. Conventional AAS has the capacity to determine more than 40 elements sequentially, generally without requiring prior chemical separation of the analyte from the bulk matrix, or other element-specific pretreatments of the sample solution. Until the introduction of the inductively coupled plasma atomic emission spectrometric (ICP-AES) technique in the 1970s, which permits simultaneous determination of many elements, AAS was the only technique for solution analysis having such an extensive capacity.

In the 1980s, the inductively coupled plasma was used as an ion source for mass spectrometry (MS) to produce another technique for solution analysis, ICP-MS, which also has the distinct advantage over conventional AAS of being a simultaneous multielement method. For AAS to remain a principal method for routine geochemical analysis in the future, it must be adapted for the simultaneous measurement of several elements.

The single element nature of conventional atomic absorption spectrometry results from the use of the hollow cathode lamp (HCL) as the light source. The lamp emits intense light exclusively at the emission wavelengths of the element used for making the cathode, hence the alternate name line source atomic absorption (AAL) for the conventional method.

While no commercial multielement AAS instruments were available as of 1986, the interest in modifying the method for multielement analysis is almost as old as AAS itself. A number of prototype multielement instruments have been described in the literature, using a number of approaches to the development of the required multielement light source.

Individual hollow cathode lamps (HCLs) are generally made for a single element. While some multielement HCLs are available, both the number of elements and the specific elements which can be successfully combined in a single cathode severely limit this approach by limiting the number of elements in comparison to AAL which might be determined by the multielement technique (Butler and Strasheim, 1965; Felkel and Pardue, 1977; Horlick and Codding, 1975; Lundberg and Johansson, 1976; Pickford and Rossi, 1973). Emission intensity for the multielement HCL is also a limitation.

Multiplexing arrangements in which the outputs of several single- or multiple-element HCLs have been largely unsatisfactory (Alder and others, 1978; Aldous and others, 1975; Chuang and others, 1978; Mavondineanu and Hughes, 1968; Salin and Ingle, 1978; Samuel and West, 1978). The complex optical arrangements required to combine the several beams generally result in light losses which reduce light throughput to unacceptably low levels. Additionally spatial considerations preclude combining more than six HCL beams, limiting the multi-element aspect of the approach.

The continuum source lamp by itself is also unsatisfactory for a number of reasons, including the requirement for a higher resolution monochromator than is typically used for AAL, and insufficient radiation throughput at UV wavelengths over the narrow wavelength range resulting from high resolution to give acceptable signal-to-noise ratios (Keliher and Wohlers, 1974). Historically AAS employed the continuum from a deuterium arc lamp for background correction (Koirtyohann and Pickett, 1965), but this lamp is not used as the primary light source. The most extensively developed of the several multielement prototype instruments, SIMAAC, uses a continuum source lamp in conjunction with an echelle grating polychromator modified for wavelength modulation (Harnly and O'Haver, 1977; Harnly and others, 1979).

This approach to multielement AAS, developed jointly by the University of Maryland and the US Department of Agriculture, was an outgrowth of the continuum source wavelength modulated atomic absorption (CWMAA) method for single element measurement (Keliher and Wohlers, 1974; Keliher, 1976; Zander and others, 1976; Messman and others, 1983). It has been the subject of two recent review articles (Harnly, 1986; O'Haver and Messman, 1986), and has been used extensively in the analysis of biological, agricultural, environmental, and geochemical samples (Harnly and others, 1982; Harnly and others, 1984; Harnly and Kane, 1984; Kane and Harnly, 1982; Lewis and others, 1984, 1985).

Recently a similar SIMAAC instrument has been developed within the Branch of Geochemistry at the US Geological Survey. This report outlines the principles of continuum source wavelength-modulated atomic absorption spectrometry and describes the system hardware. A description of the system control and data acquisition software also appears in this report. Future reports will describe the software for reducing absorbances to concentrations and for providing reports of absorbance or concentration data and will offer a procedures manual for routine operation of the instrument. Evaluation of the accuracy and precision of concentrations determined by SIMAAC methods also will be published separately.

PRINCIPLES OF CONTINUUM SOURCE WAVELENGTH MODULATED ATOMIC ABSORPTION SPECTROMETRY

The key components of SIMAAC (Simultaneous Multielement Atomic Absorption with a Continuum Source) are a 300 W xenon arc lamp, an echelle polychromator, a quartz refractor plate wavelength modulator, and a dedicated computer (Harnly and O'Haver, 1977; Harnly and others, 1979). All of the major components are available commercially and are used with little or no modification. Only the electronics for the amplification of the 20 spectrometer photomultiplier tube (PMT) signals prior to digitizing them had to be built in-house. None of these components could be substituted singly for its counterpart in a conventional AAL system to produce a successful multielement instrument. The success of SIMAAC results from the unique combination of all of these components in a way that removes the limitations imposed by simple substitution of any individual component for its counterpart in a conventional AAS instrument.

The primary light source is a 300 W xenon arc lamp (Cochran and Hieftje, 1977; O'Haver and others, 1978) which provides approximately collimated light over the entire spectral range useful for atomic absorption measurements. The arc, however, is more intense at wavelengths above 270 nm, and exhibits an instability that causes considerable flicker noise. Direct substitution of the xenon arc lamp for the HCL by itself, therefore, would cause severe deterioration of the detection limit achievable with AAL.

The broad band emission of the xenon arc lamp is also a problem when it is directly substituted for the HCL in an otherwise unchanged AAS instrument. Atomic absorption spectrometers are typically medium resolution instruments whose spectral bandpasses are several orders of magnitude wider than the approximately monochromatic HCL emission lines. The absorption of this monochromatic light by a sample solution aspirated into the flame follows Beer's Law over approximately two orders of magnitude of concentration above the detection limit. Deviations from Beer's Law at lower concentrations can result from faulty instrumentation, or from hyperfine line structure, resonance line broadening, and the ratio of the absorbtion and emission line widths (Rubeska and Svoboda, 1965).

The spectral profile for absorption by any element exceeds the width of the HCL emission line at low concentrations, and broadens considerably more with increasing concentration. Absorption of light from the xenon arc lamp will occur over the entire absorption profile width. The resulting lack of monochromaticity in the absorption region leads to significant deviation from Beer's Law, resulting in unacceptable calibration curvature and degradation of characteristic concentrations in comparison to AAL.

Measurement in continuum source AAS can be made essentially monochromatic by using a high resolution spectrometer. Echelle spectrometers provide the required high resolution. Additionally, an order-sorting prism used in conjunction with an echelle grating provides a polychromator with up to 20 exit slits, each having its own dedicated detector (Keliher, 1976; Keliher and Wohlers, 1976). Thus, an echelle spectrometer begins to meet the requirements for a successful multielement AAS system.

The emission from a xenon arc lamp has already been noted to be weak below 270nm. Also, light throughput by the echelle configuration is low compared to that of conventional AAS because high resolution requires the use of narrower entrance slits. These facts, coupled with the high flicker component of the xenon arc emission, still result in an unsatisfactory signal-to-noise ratio for AA measurements.

Modification of the echelle spectrometer for wavelength modulation at a frequency, f, which exceeds the 50Hz frequency of the lamp flicker, remedies the problem (Snelleman, 1968). It also provides for intrinsic background correction (Harnly and O'Haver, 1977), and by taking advantage of the absorption of light over the entire width of the absorption profile, an extension of the calibration range from one and a half to two orders of magnitude (typical of conventional AAS) to about 6 orders of magnitude becomes possible (Harnly and O'Haver, 1981).

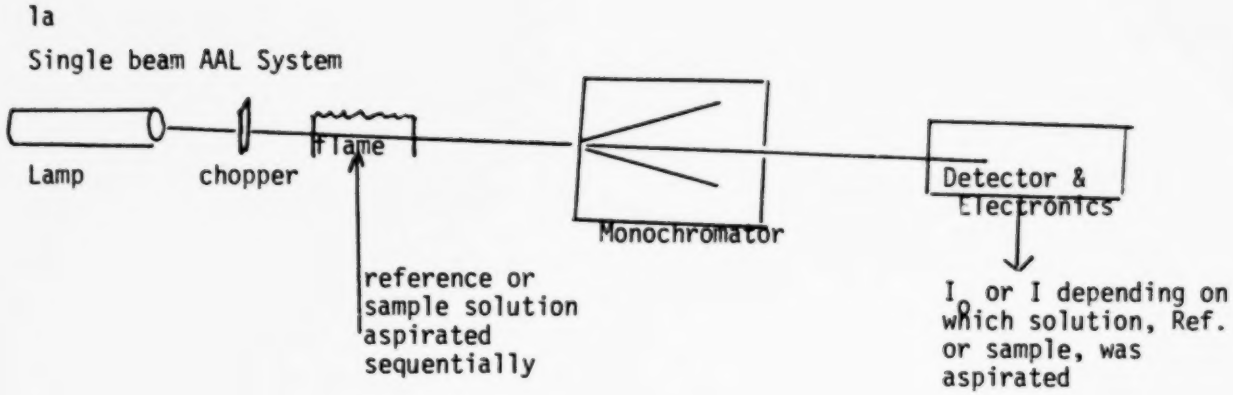
The modification to enable wavelength modulation is readily accomplished by mounting a 3mm- or 6mm-thick quartz refractor plate on a galvanometer just behind the entrance slit. A computer-generated signal input through the scanner controller drives the galvanometer. The specific waveform used and the modulation frequency are under software control.

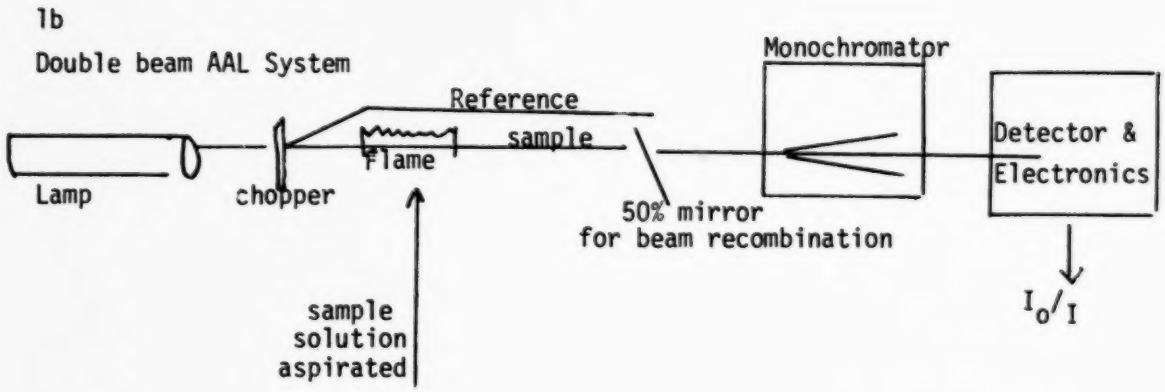
Computation of absorbance (A) is made using equation (1)

$$(1) \qquad A = -\log (I_o/I)$$

where I_o and I are the source lamp intensities prior to and after absorption, respectively. In conventional AAL, I_o and I are measured along different light paths, one of which does not pass through the absorption cell (double-beam instruments), or at different times (single-beam instruments), as shown in Figures 1a and 1b. The measurement is not intrinsically background corrected. The original approach to such correction (Koirtyohann and Pickett, 1965) alternately measures absorbance of a spectral line emitted by an HCL and absorbance of the output from a continuum source. The background-corrected absorbance then is the difference between the total (HCL) and background only (continuum) absorbances. Accuracy of this correction requires exact superposition of the HCL and background lamp beams and equal intensities of the two.

Figure 1 Optical Scheme for AAL Measurement of I_o and I





With wavelength modulation, the reference/background absorption measurement, I_o, and the sample absorption measurement I are made almost simultaneously at slightly different wavelengths along the same light path (Figure 2). And unlike double-beam AAL, both are measured in the absorption cell. The actual time lapse between measurement of I_o and I will never exceed 1/f, and depends on the specific positions within the modulation interval at which the two intensities are measured. A detailed discussion appears in the later section on software. At this point note that I_o in SIMAAC is measured off the absorption line center, and that background correction is intrinsic to this method. This is also true of Zeeman and Smith-Hieftje approaches to background correction (Hadeishi and McLaughlin, 1976; Brown, 1977; Smith and Hieftje, 1983; Sotera and Kahn, 1982).

Furthermore, any number of off-line measurements of I, in addition to the measurement directly on-line, can be made within the modulation interval. Thus, computation of a series of background-corrected absorbances, defined by equation (1a), having successively decreasing sensitivities is possible (Harnly and O'Haver, 1981), where I_n is measured at increasing distances from the profile center.

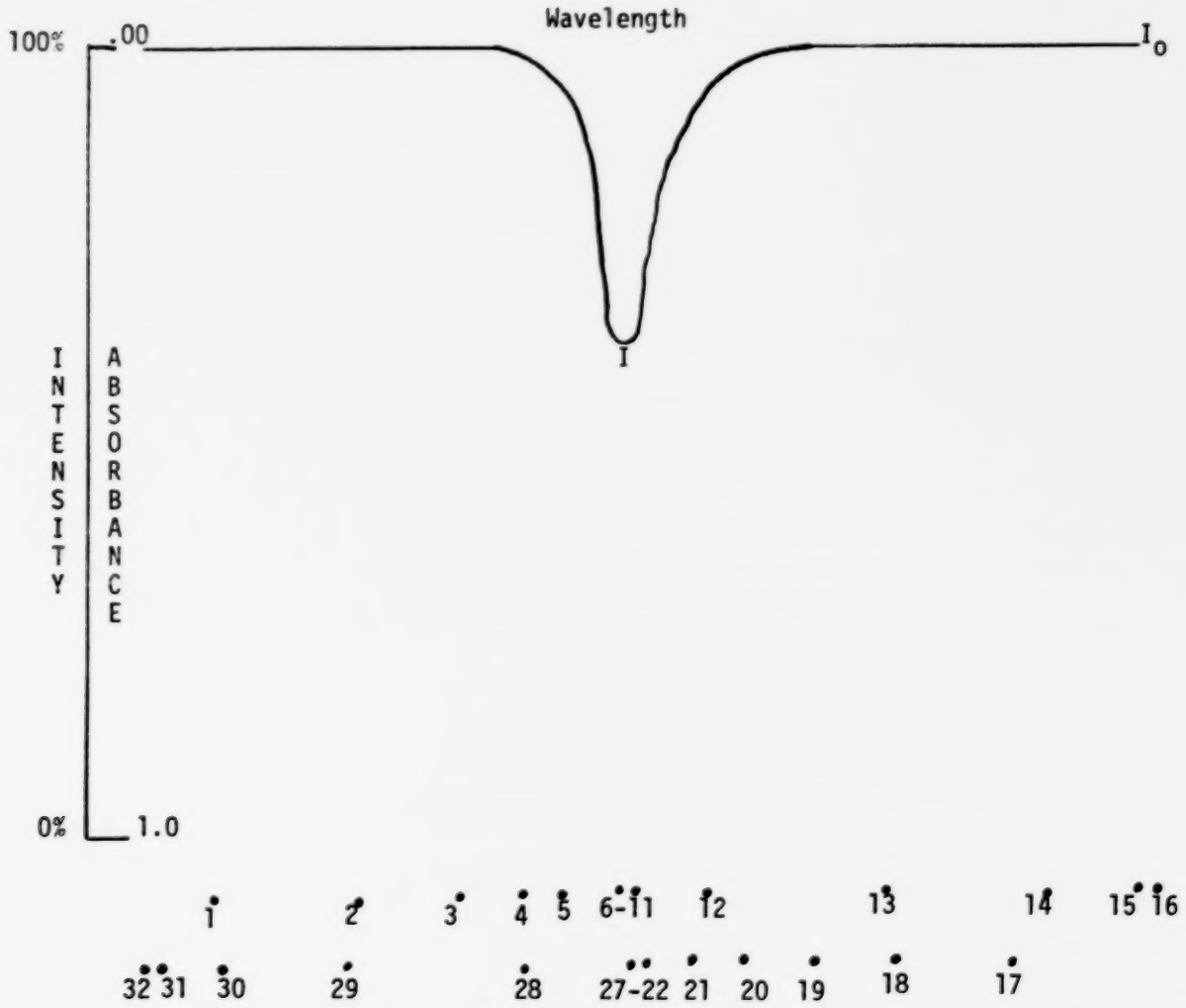
$$(1a) \qquad A_n = - \log (I_o/I_n)$$

While the calibration range for AAL can be extended by burner rotation or by use of alternative measurement wavelengths, either approach requires repetition of the measurement at the newly defined experimental conditions. The extension of the SIMAAC calibration range is inherent in the modulation process, and occurs for all elements under software control, in a manner to be discussed later in the software section of this report.

Calculation of the series of absorbances given by equation (1a) for each of several standard solutions leads to a family of calibration curves, as shown in Figure 3. No one curve covers a larger concentration range than is observed in AAL, but because each is displaced relative to the preceding one along the concentration axis, the range is extended by using successive curves as the concentration increases. Also none of the curves is linear over its full calibration range, but the application of a variety of curve-fitting approaches provides concentration data beyond the linear ranges of these calibration curves (Miller-Ihli and others, 1984a). For all but the least concentrated samples, concentrations will typically be extrapolated from more than one curve, because the ranges for these curves overlap.

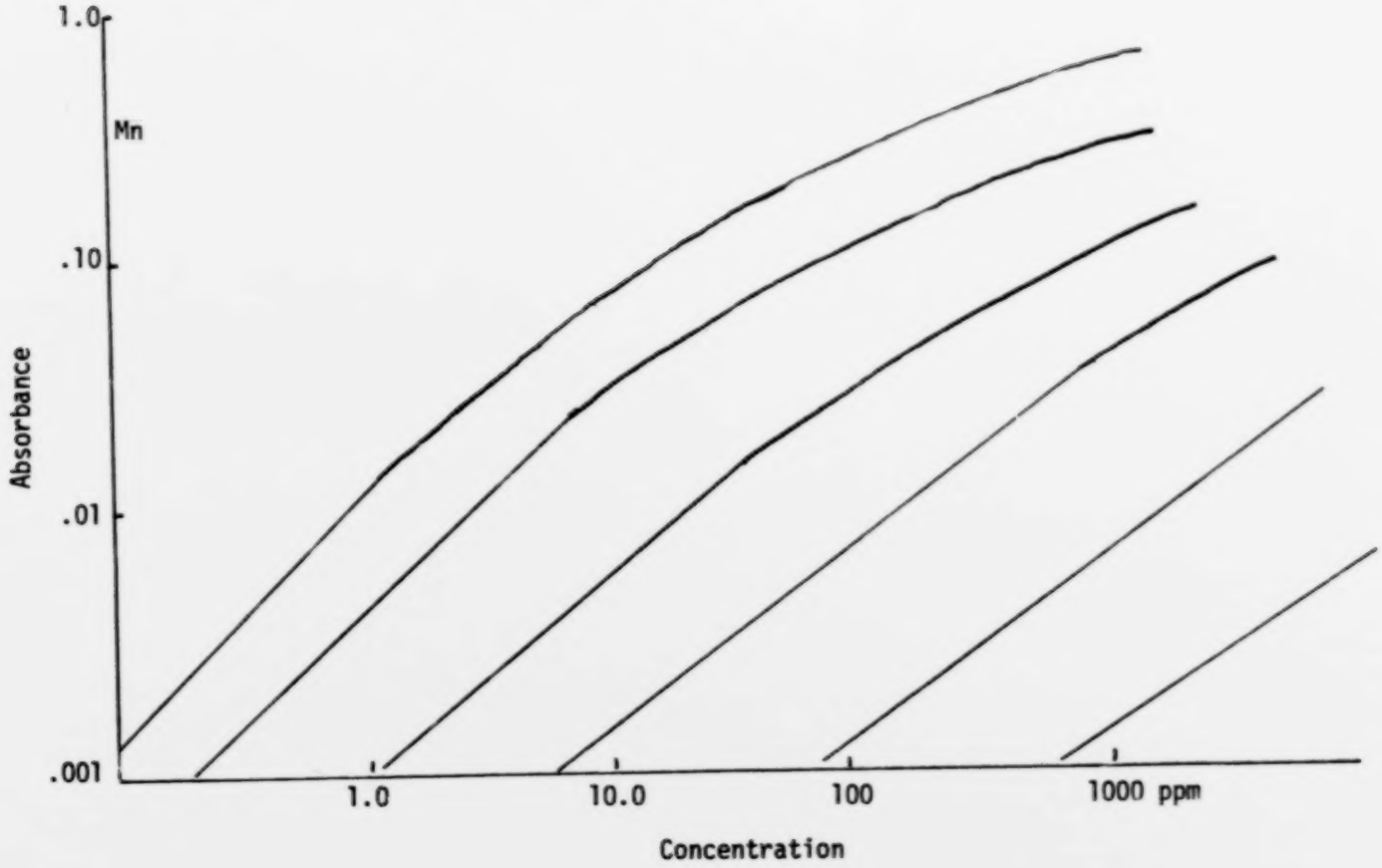
The shape of these calibration curves is determined by two factors. First, some curvature is expected due to the non-monochromaticity of the absorbed light. This curvature results from the use of a continuum source , and from the measurement of intensities at more than one refractor plate position in establishing the I_n values used in the absorbance calculations. The degree of non-monochromaticity is determined by the entrance slit used for the echelle spectrometer, and by the width of the

Figure 2 Optical Scheme for SIMAAC Measurement of I_o and I



Individual points for intensity measurement within the modulation interval

Figure 3 SIMAAC Family of Calibration Curves



modulation interval. Narrowing the entrance slit or modulation interval reduces the spectral bandpass for the echelle spectrometer, and increases the between-point wavelength resolution (or monochromaticity of each measured intensity) across the interval.

The absorbance limit of linear dynamic range is determined by the ratio of the width of the spectral bandpass of the spectrometer to the width of the absorption profile. Since this ratio changes with increasing concentration as the profile broadens, the absorbance at which curvature is first noted decreases from curve 1 to curve 6.

Far stray light is common to most spectrometers, and is most significant in the far UV; it can cause a decrease in the linear range. This effect can be greatly reduced by using solar blind PMTs for analytical wavelengths below 230nm. An additional source of stray light from order overlap is specific to the echelle spectrometer. It arises from incomplete separation of orders by the prism, is insignificant below 450nm unless slit heights greater than 300 μm are used, and increases with wavelength. Its severity is compounded for SIMAAC because source intensity also increases with wavelength. However, none of the analytical wavelengths used on the USGS instrument at present exceed 450nm, and thus order-overlap stray light may be ignored.

It should also be noted that the absorbances calculated according to equation 1a for the blank are frequently negative, because the blank absorbance profile bows downward at the modulation interval extremes. This results from two factors. First, incident light lost by reflection off the refractor plate is greater at the large angle of rotation at the end point than at the midpoint of the rotation interval. Additionally, modulation occurs in a horizontal plane, while orders have a 9° slope to the horizontal plane (Harnly and O'Haver, 1981).

HARDWARE

The hardware components that make up the SIMAAC system are described in Table I, and a block diagram of the instrument appears in Figure 4. The discussion which follows focuses on interfacing the several components properly to build a functional multielement atomic absorption instrument.

The Spectraspan III echelle grating spectrometer is manufactured as part of a DC plasma emission system, which consists of a DC plasma excitation source and a microprocessor system including a control panel, in addition to the spectrometer (Spectrametrics, Inc.). For use as a component of SIMAAC, the Spectraspan III spectrometer alone is used. Its baseplate is modified by removal of a section in front of the PMT housing and to the right of the entrance slit to provide space for mounting the atomic absorption atomizer (flame or graphite furnace) in front to the entrance slit. Both a flame and a graphite furnace atomizer are desirable as interchangeable absorption cells that can be mounted on the optical rail. Power supplies are needed to provide 30V to the step-up transformer for the PMT tubes and 5V to the instrument panel LEDs, which is otherwise provided by the

Figure 4 Block Diagram of SIMAAC Hardware

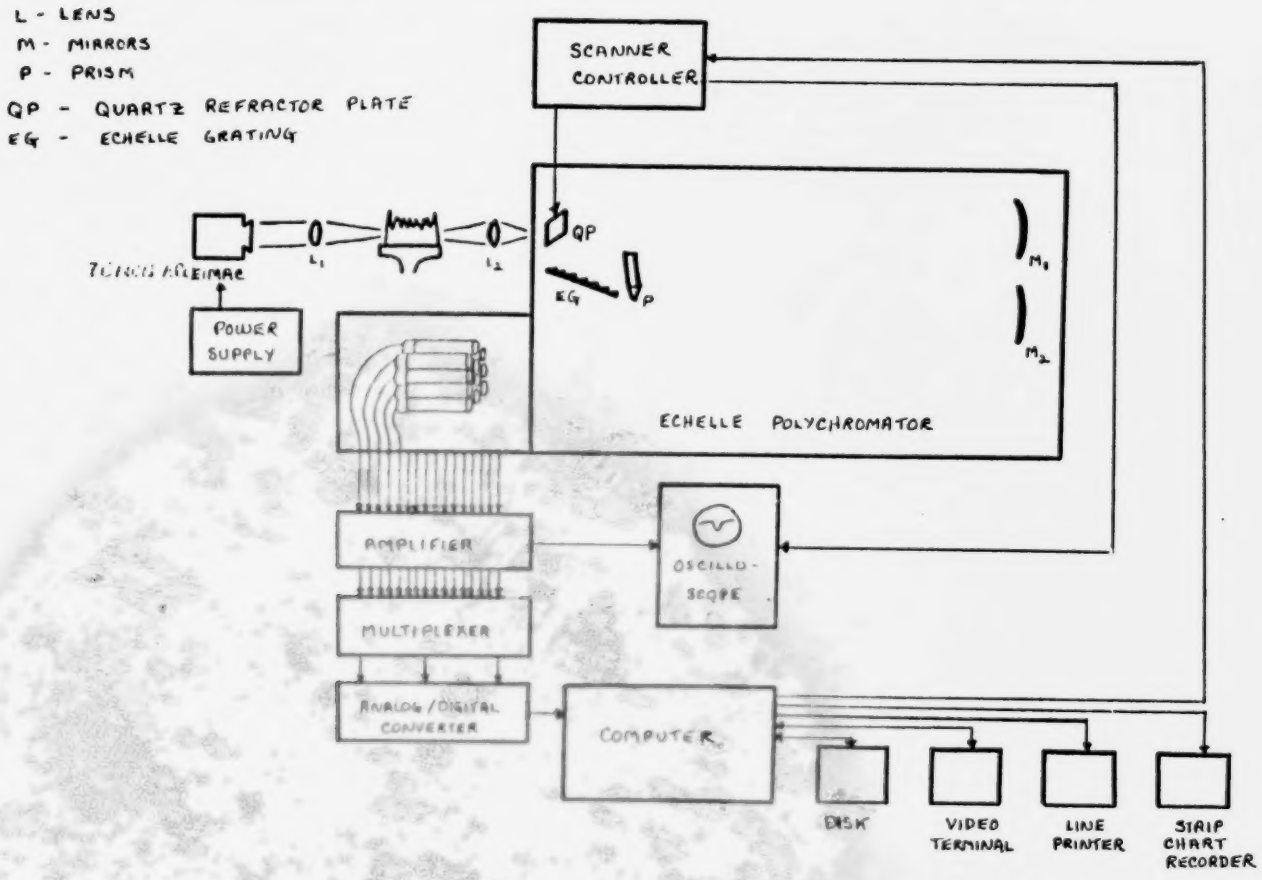


TABLE I INSTRUMENT HARDWARE

Component	Model	Supplier	
Xenon Arc Illuminator	Model LX300 UV	ILC Technology Sunnyvale, CA	
used with			
lamp holder	Model R-300-3		
power supply	PS 300-1		
Echelle Spectrometer	Spectraspan III B	Applied Res. Brea, CA	echelle grating with order sorting prism adjustable entrance slit aperture, 25,50,100,200 μm width 100,200,300,500 μm height a single slit exit slit casette with comparable adjustable slits a 20-channel multislit exit slit casette fixed at 50x300 μm R292 Hammamatsu PMT tube detectors powered by high voltage supply, variable from 550 to 1000V in 50V increments reciprocal linear dispersion 0.062 nm at 200 nm and 0.250 nm at 800 nm spectral bandpass 0.0015 nm at 200 nm and 0.0600 nm at 800 nm
Scanner Controller	CCX101	General Scanning Watertown, MA	
Galvanometer	G300PD		
Computer	PDP 11/34	Digital Equipment Landover, MD	with CRT, printer, 2 RL01 disk drives and add-on boards: AA11-K digital to analog converter- 4 channels AD11-K analog to digital converter- 16 channels DR11-K input/output board KW11-K real time programmable clock and using RT11 operating system having FORTRAN available
Atomizer	HGA 400 Burner Controller and AA Burner Assembly for P-E 603 spectrometer	Perkin Elmer Norwalk, Conn.	

microprocessor-instrument control panel. The required connections are shown in Figure 5a, as viewed from the solder side of the bulkhead connector located at the back of the spectrometer baseplate. The galvanometer required for the wavelength modulation is not the one used for the optional background correction module of the Spectraspan III. Rather, it is a replacement that allows external control of the modulation waveform. Neither the galvanometer mounted in our spectrometer, nor the controller used to drive it, are available any longer from the manufacturer. Newer models are available which function identically, but which combine in a single 15-pin connector the 2-pin power and 5-pin position connections of the older models.

The 3mm-thick quartz refractor plate is mounted on a fitting which slips over the shaft of the galvanometer, and is held in position with a set screw. With the galvanometer in position on the internal baseplate of the spectrometer, the refractor plate should be exactly parallel to the plane of the entrance slit. This assures that the rest position is at the center of the waveform, and corresponds to 0^{o} rotation of the plate.

For initial testing of wavelength modulation and for field alignment of the exit slits, a function generator was used to input a sine wave to the galvanometer through the scanner controller. Although the sine wave is adequate for these purposes, of the three waveforms evaluated for SIMAAC measurement of absorbance (Harnly, 1982), it produces the least sensitive absorbance signal, and is therefore not used for measurement purposes.

For the absorption measurements, a bi-Gaussian or other appropriate waveform (Harnly, 1982; Miller-Ihli and others, 1984b) is generated under software control. The waveform voltages are generated as AA11-K digital-to-analog converter (DAC) board (Digital Equipment Corp., 1976b) outputs and are used as external input to the scanner controller. Connections are made through an H232 distribution panel and BC08R cable. Terminal and pin assignments are shown in Table IIa. Maximum external input range to the scanner controller is $\pm$ 2.5V, producing $\pm 25^{o}$ rotation of the refractor plate. (Harnly and O'Haver, 1981; Miller-Ihli and others, 1982). The attenuator control allows adjustment for a smaller angle of rotation of the plate. The rotation angle determines the width of the modulation interval in nanometers, as given by equation (2).

$$(2)\quad \Delta\lambda = (dl/dx)T\phi(n-1/n)$$

where $\Delta\lambda$ represents the modulation interval,
dl/dx represents the reciprocal linear dispersion in nm/mm for the order of the wavelength of interest
T is the thickness of the refractor plate (3mm)
ϕ is the angle of rotation in radians of the plate
and n is the refractive index of quartz.

Figure 5a Schematic of Power Supply Connections to Bulkhead Connector

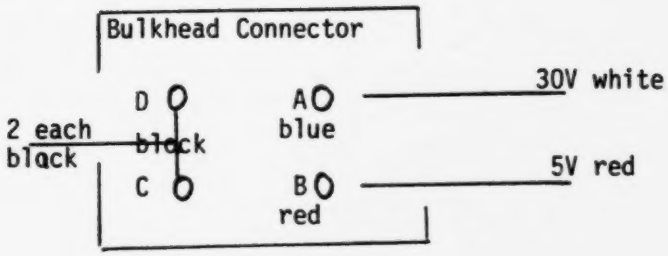


Table IIa

Pin and Terminal Assignments for DAC Connections

Terminal Strip	Pin	Connection	
J1	J	0 HQ ground	to scanner
	K	DA 0 out	to scanner
	R	2 HQ ground	to recorder
	W	DA 2 out	to recorder (optional)

Table IIb

Pin and Terminal Assignments for ADC Connections

Terminal Strip	Pin	Connection
J9	VV	ADC channel 0*
	TT	ADC channel 1
	KK	HQ ground
	RR	ADC channel 2
	NN	ADC channel 3
J8	LL	ADC channel 4
	JJ	ADC channel 5
	EE	HQ ground
	FF	ADC channel 6
	DD	ADC channel 7
J7	BB	ADC channel 10
	Z	ADC channel 11
	AA	HQ ground
	X	ADC channel 12
	V	ADC channel 13
J6	T	ADC channel 14
	R	ADC channel 15
	W	HQ ground
	N	ADC channel 16
	L	ADC channel 17

* Channels for programming purposes are numbered in octal, beginning with 0. That numbering is used in this table, and in appendix 1a, but not in most of the discussion, where channels are numbered 1-16, decimally.

The H322 panel decal which identifies positions on the terminal strip follows the Table as Figure 5b.

Figure 5b H322 Terminal Strip Connections

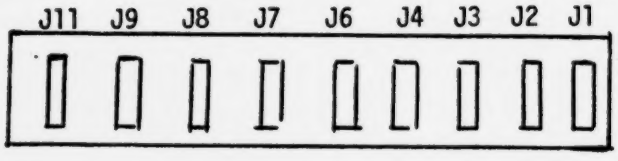
H322 DAC

J4	J3	J2	J1	
PP	C	D	F	
SS	H	B	M	
OO	E	P	J	OHQ ground to scanner
S	A	U	K	DAO out
MM	HH	CC	Y	
VV	LL	BB	T	
TT	JJ	Z	R	2HQ ground to optical recorder
KK	EE	AA	W	DA2 out
RR	FF	X		
NN	DD	V		

H322 ADC

J9	J8	J7	J6
PP	C	D	F
SS	H	B	M
UU	E	P	J
S	A	U	K
MM	HH	CC	Y
VV ch0	LL 4	BB 10	T 14
TT ch1	JJ 5	Z 11	R 15
KK HQgrnd	EE HQgrnd	AA HQgrnd	W HQgrnd
RR ch2	FF 6	X 12	N 16
NN ch3	DD 7	V 13	L 17

H322

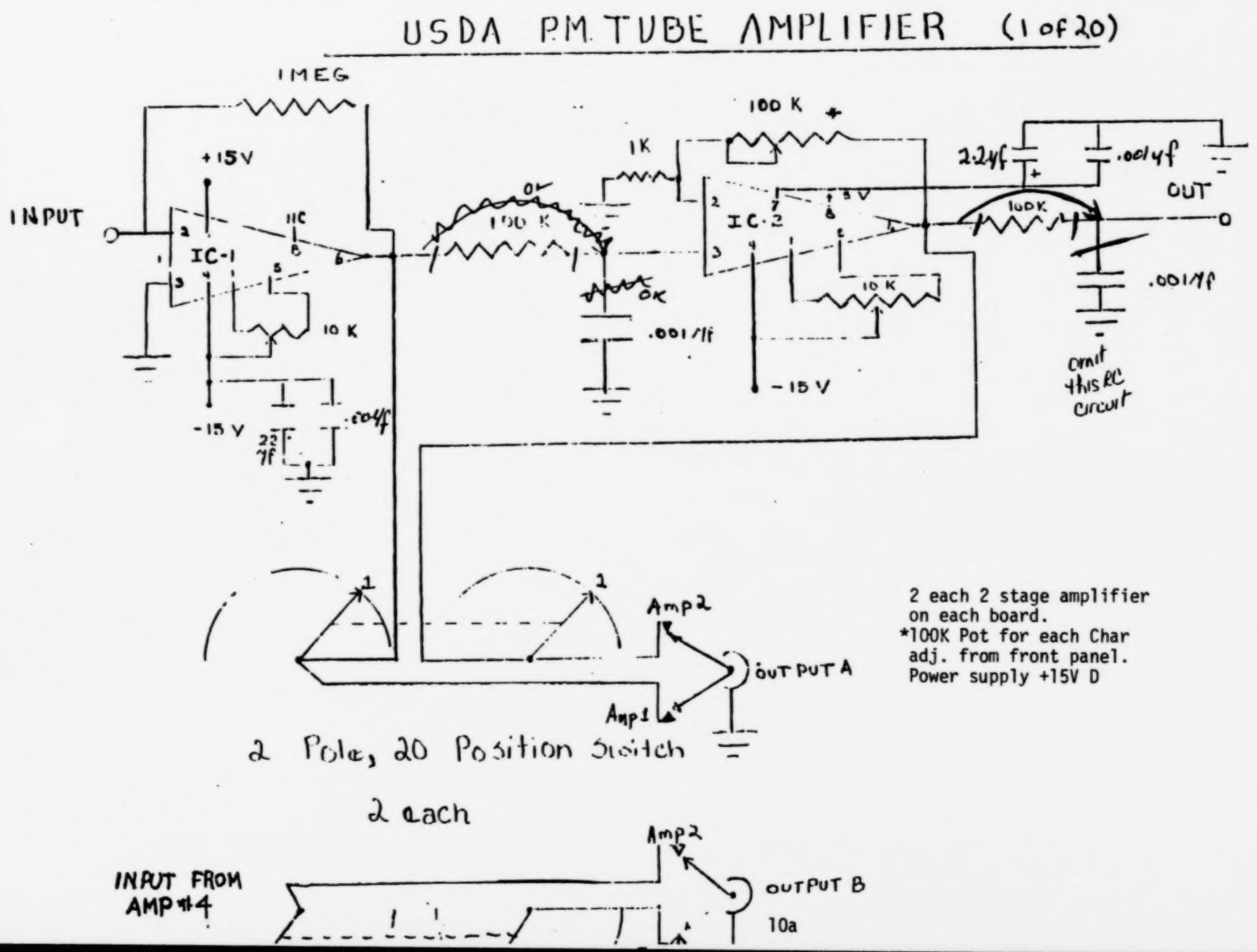


This modulation interval will vary from element to element, depending on the order in which the analyte wavelength falls. The echelle polychromator uses a small wavelength segment from each of the orders 28 to 128. The reciprocal linear dispersion is different for each order, being highest for the order used for the lowest wavelength. The timing for generation of the voltage waveform and for data acquisition is controlled by the KW11-K programmable clock (Digital Equipment Corp., 1976c). The DR11-K input-output board (Digital Equipment Corp., 1975) generates an interrupt to trigger the onset of modulation and data collection at the start of sample atomization with a transition from 5 to 0V at the external input position. This transition occurs for flame atomization when a foot peddle switch is activated by the analyst. The 5V is supplied to the foot-peddle circuit by a parallel connection to the same 5V supply powering the spectrometer LEDs. For furnace atomization, the HGA-controller "record signal" generates the interrupt to begin modulation and data collection. The connections are made directly to the external input 4 of the board through the BC08R cable at position J1. The foot pedal and furnace record signals are connected at cable pins NN and RR and earth ground is connected to pins SS and UU.

For alignment of the exit slits, a one-time operation at the time of spectrometer installation, the PMT signals are displayed directly on an oscilloscope. Processing the signals for the absorbance calculations requires preamplification and digitization. For this, preamplifier circuits designed by J. Harnly for the USDA instrument (Harnly and O'Haver, 1977) and later modified to eliminate cross talk between adjacent channels (Miller-Ihli and others, 1982) were built in the USGS electronics shop by D. Dotson. Figure 6a gives the circuit diagram of one of these preamplifiers. Two circuits are built on a single plug-in circuit board; ten boards are required for the SIMAAC system. Connections between these circuits and the individual channels of the computer AD11-K ADC are made through the H232 distribution panel with a standard BC08R cable. Terminal assignments for this distribution panel and corresponding pin assignments for the cable are given in Table IIb.

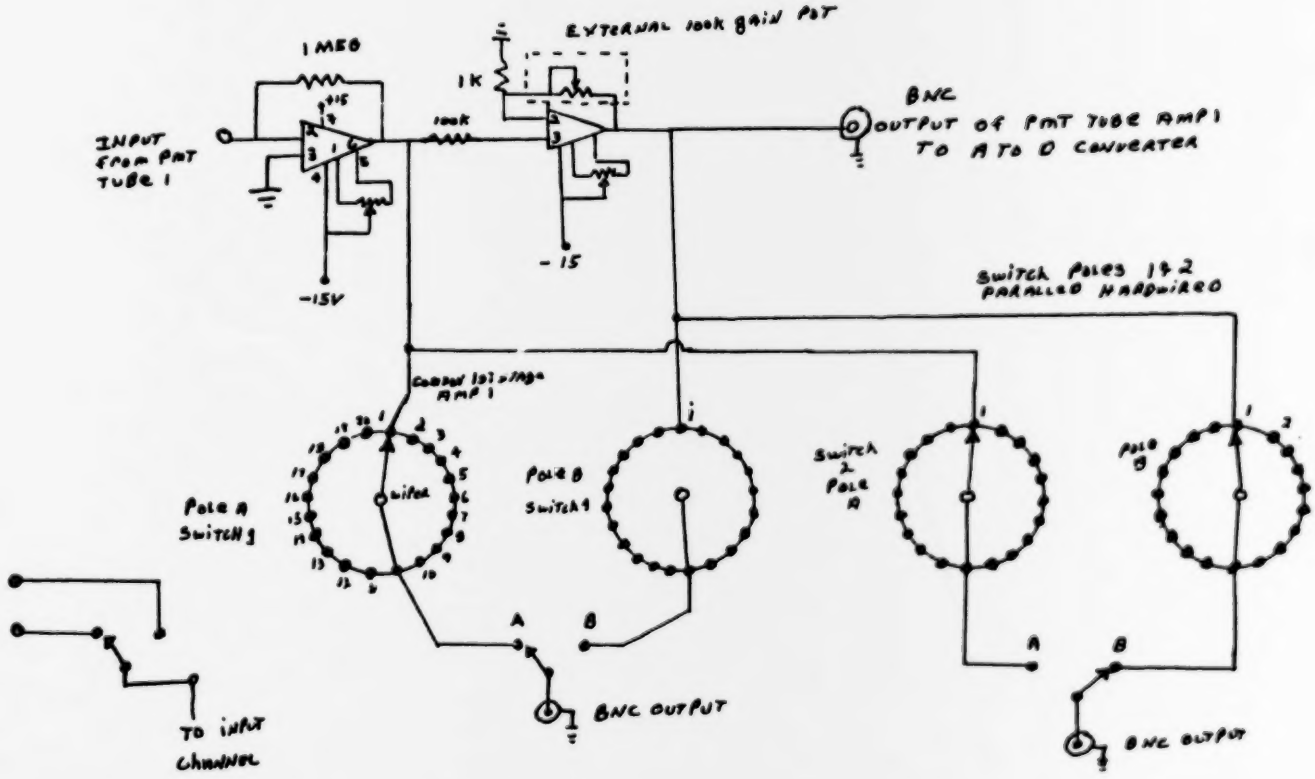
For the USGS SIMAAC instrument, the circuit boards for preamplification of the 20 PMT outputs are mounted in a switch box (Figure 6b) which permits selection of any two outputs for monitoring on an oscilloscope at the same time that they are being acquired by the ADC. Switching on the box also permits examination of the unamplified PMT input to each of the circuits. The gain of each circuit is variable through a ten-turn potentiometer on the switch box, while the dynode gain of the PMT is increased or decreased by varying the voltage to the PMT using a 10-step thumbwheel switch located on the PMT housing. For optimum signal-to-noise ratio in the absorbance measurement, the lowest PMT voltage is used which will provide an input adjustable with the circuit gain to the full 10V range of the ADC. Since the spectrometer has 20 exit slits, but the ADC has only 16 channels, another set of switches allows easy selection, for the four pairs of exit slits, as to which in each pair will be processed by the ADC.

Figure 6a Preamplifier Circuit Diagram



2 each 2 stage amplifier on each board.
*100K Pot for each Char adj. from front panel.
Power supply +15V D

Figure 6b Switch Box Diagram (D. Dotson)



Dual 2 stage current amplifier with DC offset and external gain
2 sets of parallel switches for viewing and adjustment outputs to
A to D converter board in deck computer.

The wavelengths isolated by the multielement exit slit casette are listed, along with their modulation intervals, in Table III. Figures 7a and 7b show the placement of slits on the casette, and in the PMT honeycomb array. In many geochemical applications, only 6 of the potential analytes (Cu, Co, Mn, Ni, Pb, Zn) will generally be detectable using flame atomization, and in the analysis for the platinum-group elements (PGE) by fire assay, only 5 of the potential 20 elements will be present in a sample solution. Based on these considerations, the switch pairing, which is also listed in Table III, was chosen such that neither two flame-detectable elements nor two PGE elements would constitute a pair. Such pairing would make measurement of the two mutually exclusive.

The xenon arc lamp and the selected atomizer are located on the optical rail and positioned for optimum transmitted light. The lamp intensity was previously noted to be a function of wavelength, and to be lowest in the UV region below 270nm. Additionally, neither the lamp output beam nor the flicker component of the beam are spatially homogeneous with respect to wavelength (Cochran and Hieftje, 1977; O'Haver and others, 1978). The optimum lamp position, thus, differs from one element to another, and should be chosen to minimize the degradation of sensitivity in comparison to single-element AAS. The degradation results from multielement compromise measurement conditions or from minor misalignments of the elements with respect to one another on the multielement casette.

Mounted externally on the spectrometer baseplate is a lens which focuses the image of the midpoint of the atomization volume onto the spectrometer entrance slit. Also, a lens is required to focus the Xenon arc output on the midpoint of the atomization volume. A 50.8mm diameter calcium fluoride lens with a 200mm focal length is used for this purpose.

The atomizers used are a Perkin-Elmer premix burner assembly and gas control unit for a Perkin Elmer model 603 spectrometer, and a Perkin Elmer model 400 heated graphite atomizer (HGAA), which mount interchangeably on the optical rail. Any similar atomizer can be substituted.

SOFTWARE

Software developed for the SIMAAC instrument consists of programs written for instrumental control, data acquisition, and data processing functions. In broad overview, the control functions involve sending the modulation-waveform voltages to the scanner controller under timer control while simultaneously collecting intensity data from each of the photomultiplier tubes, and storing that data on disc for subsequent reduction. The primary data processing functions involve first time-averaging or integrating the intensity data collected over the modulation interval, depending on whether flame atomization or furnace atomization was used, and then transforming that intensity data into absorbances. Additionally, the absorbances can be curve-fit to produce concentration data, plotted to provide absorbance profiles, or reported in a number of other ways.

Figure 7a Slit Positioning on Multielement Exit Slit Cassette

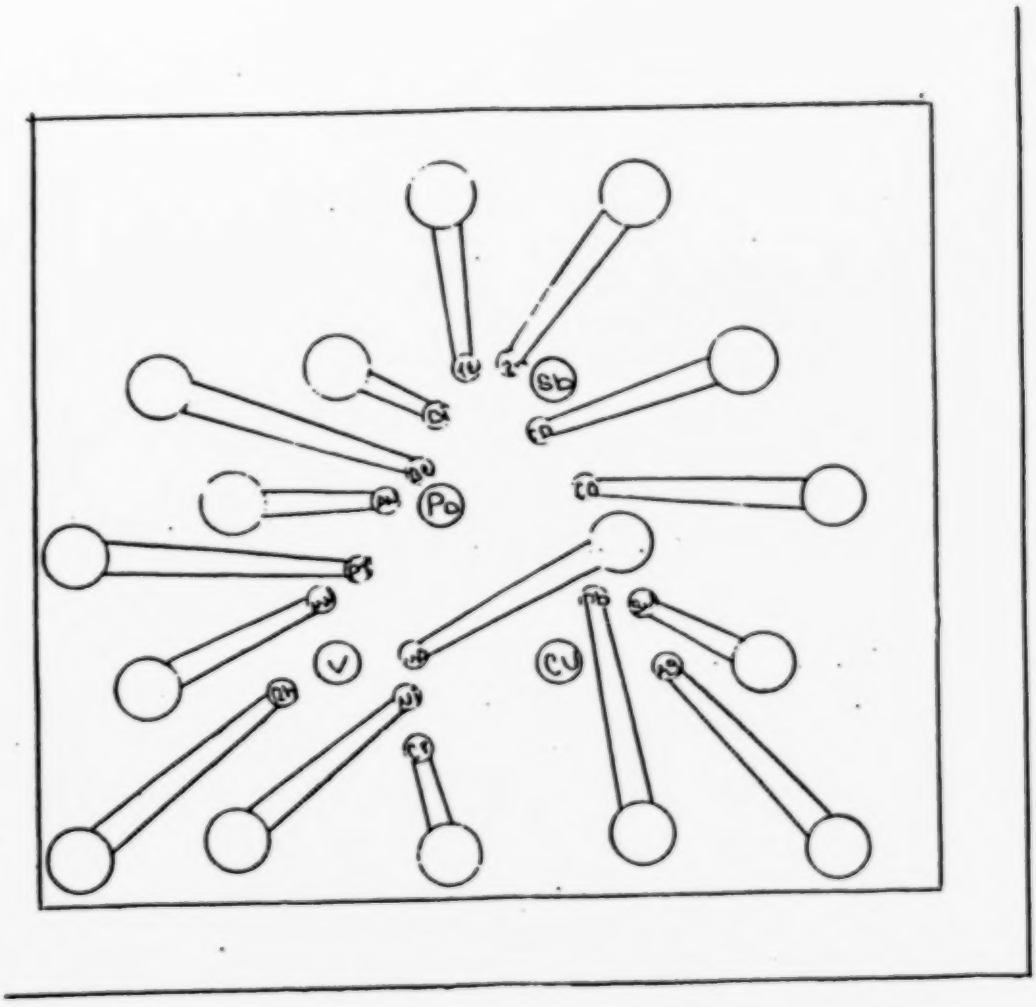


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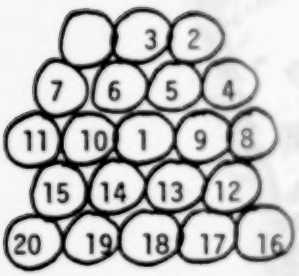
Figure 7b

PMT Positions in Honeycomb Array



1 = Single channel or Pd
2 = Zn 7 = Be 12 = Sn 17 = Pb
3 = Te 8 = Co 13 = Cu 18 = Cr
4 = Cd 9 = Mo 14 = V 19 = Ni
5 = Sb 10 = Au 15 = Mn 20 = Rh
6 = Bi 11 = Pt 16 = Ag

Table III

Element	Wavelength in nm	Modulation Interval in nm	Spectral Bandpass* in nm	PMT	Paired with	ADC channel
Pd	244.91	0.067	0.0019	1	3	1
Zn	213.86	0.058	0.0016	2	-	2
Te	214.28	0.058	0.0016	3	1	1
Cd	228.80	0.062	0.0017	4	-	3
Sb	217.58	0.059	0.0016	5	11	4
Bi	223.06	0.060	0.00165	6	-	5
Be	234.86	0.064	0.00175	7	-	6
Co	240.73	0.066	0.0018	8	-	7
Mo	313.26	0.086	0.0023	9	-	8
Au	242.79	0.067	0.00185	10	18	9
Pt	265.95	0.73	0.0020	11	4	3
Sn	286.33	0.078	0.00215	12	-	10
Cu	324.75	0.090	0.00245	13	-	11
V	318.54	0.088	0.0024	14	-	12
Mn	279.48	0.076	0.0021	15	20	13
Ag	328.07	0.090	0.0025	16	-	14
Pb	283.31	0.078	0.00215	17	-	15
Cr	425.54	0.115	0.0034	18	10	9
Ni	352.45	0.097	0.00265	19	-	16
Rh	343.49	0.096	0.00265	20	15	13

* Spectral bandpass is given for 25 μm entrance slit width.

The individual functions for instrument control and data acquisition are the following, listed in order of execution:

1) initiation of modulation and data acquisition on receipt of an interrupt by the DR11-K I/O board,

2) timer control of the modulation waveform and data acquisition by the KW11-K real time clock,

3) actual waveform voltage output to the scanner controller from the AA11-K digital to analog converter (DAC),

4) rapid sequential sampling of the photomultiplier tube outputs from the multiplexed 16 channel AD11-K analog to digital converter (ADC),

5) real time storage of up to 14,000 words per second of data acquired continuously for 10 seconds per sample on RL01 disc.

The primary data manipulation task, reduction of the raw data to as many as 6 computed absorbances per active channel, is also performed in real time, between samples, by the instrument control and data acquisition program. The program, in two slightly different versions for flame and furnace atomization, is written in FORTRAN, although only the experimental setup and final computation of absorbances are coded in that language. The heart of the control and data acquisition functions are coded in MACRO to provide the needed execution speed for modulation at 56Hz and data acquisition and storage without loss of any data.

The discussion which follows examines in detail each of the control functions. Initially, each control function was programmed and tested independently of all others, in an order quite different from the final execution sequence. Only after each function was found to be independently operational, were the MACROs linked and converted to a subroutine that can be called by the FORTRAN main program.

The first function tested was the analog-to-digital conversion of the PMT tube output. The AD11-K board (Digital Equipment Corporation, 1976a) can provide any of three ranges of output, depending on user installation of jumper W4. SIMAAC uses the 0-10.24V output range for optimal resolution of small intensity changes. Voltages can be input directly from a 10V variable power supply to individual terminals of the distribution panel, and conversions started by depositing the appropriate start bit for the channel in the status register for the board from the computer front panel. Examination of the status register should then show the stop bit , and examination of the buffer register will show the converted value representing the input voltage. Full scale conversion of 10 V results in a digital value of 7777 (octal) for the 12-bit converter. The PMT output gains must be set so that the light throughput in the absence of absorbing sample never exceed this full scale output value, so that small baseline absorbances can indeed be measured. It is advantageous, however, to use as much as possible of the full 10 V range of the ADC to minimize quantitation noise in the

measurement of changing intensities. Order misalignment between elements on the multiple-element exit slit casette can cause some reduction in useable range. Details of output gain optimization will be given in the procedures manual for routine operation of the instrument.

The program ADTEST samples all 16 channels repetitively, performing a conversion on each in sequence, buffering the conversions in memory and outputting the data to the CRT. Using voltages applied to only some of the channel terminals, and knowing expected octal outputs for given voltage inputs, one can verify that each channel is functioning properly. The program listing and typical input-output listings are given in Appendix 1a, along with a flow diagram of the program logic and a table of the start and stop bits for each channel.

Next to be programmed was a simple test of the AA11-K board (Digital Equipment Corporation, 1976b). The program AATEST repeatedly output a series of voltages, one after another, to the scanner controller. Rather than driving the galvanometer with the controller output for this test, the voltages were observed on an oscilloscope. This procedure allowed verification of the board function and setting of the scanner controller offset and attenuation so that the full $\pm$ 5V output range of the board could be used for maximum positional accuracy without exceeding the maximum $\pm$ 2.6V range of the galvanometer input. In the first version of the program, the series of voltages simply ranged from -5V to +5V in steps of approximately 0.5V. This version of the program and accompanying logic diagram is given in Appendix 1b. Later the 40 voltages of the bi-Gaussian waveform used for the SIMAAC instrument at USDA were used (Miller-Ihli and Harnly, 1983), and the entire voltage table was cycled through 100-200 times.

When using this program, output of the scanner controller could be examined on the oscilloscope to verify the shape of the waveform (Figure 8a). Alternatively, the scanner output was used to drive the galvanometer and the x axis of an x-y oscilloscope. At the same time, a sample solution was aspirated. The output from one of the PMTs (or ADC channels) was input to the y axis of the scope to observe the absorbance profile for the sample solution (Figure 8b). A third option used output voltages from the scanner controller as input to one channel of the ADC. For this, the controller offset had to be adjusted to shift the 5V DAC output into the ADC 0-10V range. Positional inaccuracy for the modulation waveform was found to be no more than 2 ADC conversion units. Recall that 7777 units (octal) corresponds to the modulation interval (Table III) which varies from 0.058nm for Zn to 0.115nm for Cr, and that the spectral bandpass for each line is considerably smaller. The positional error in waveform generation is at worst 0.00015nm or less than 10% of the spectral bandpass.

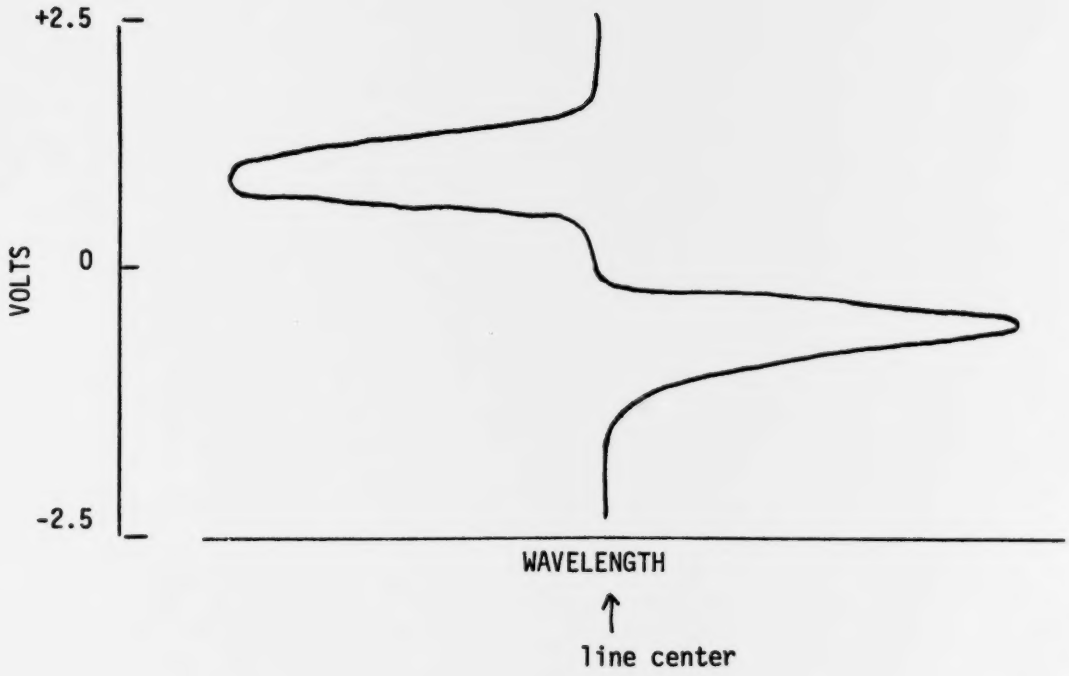
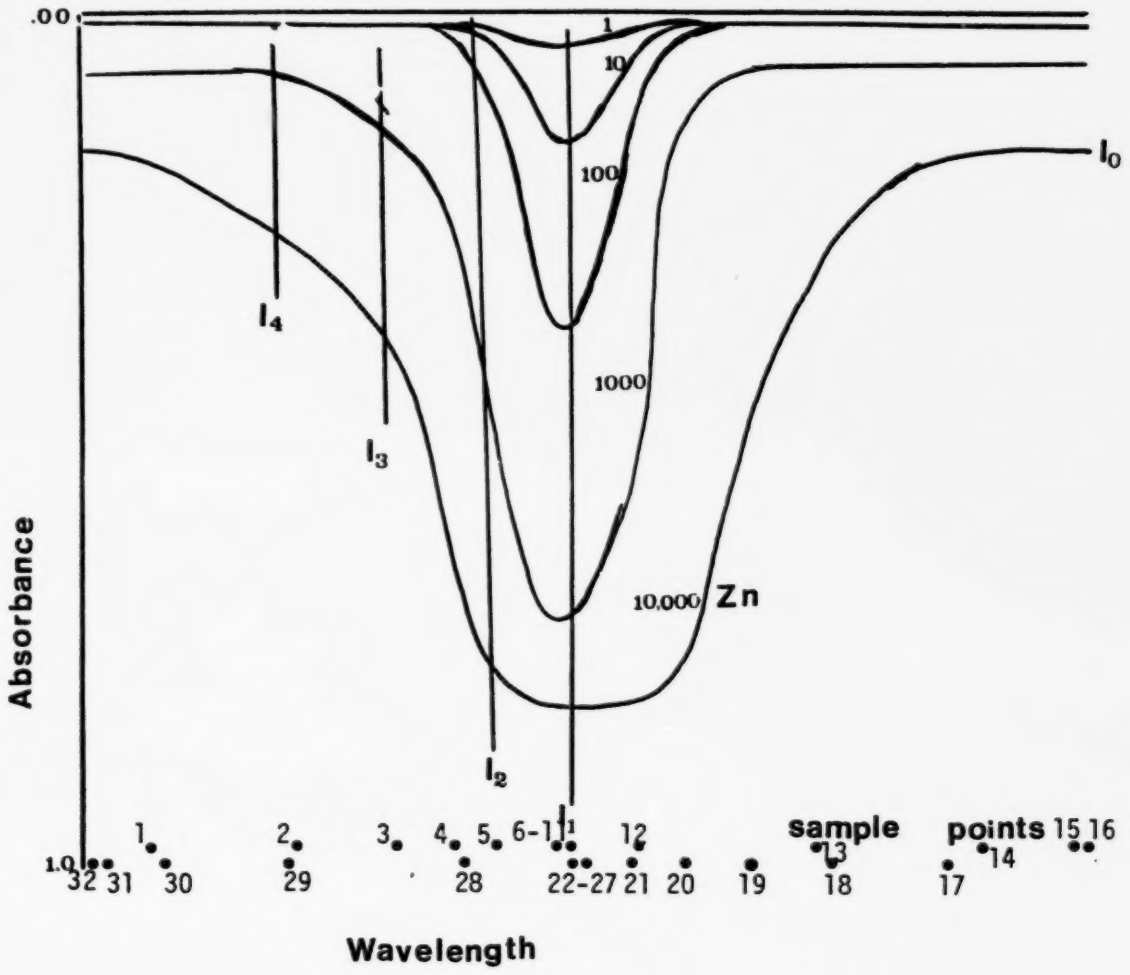


Figure 8a SIMAAC Modulation Waveform

Figure 8b Simaac Absorbance Profile



Finally an edit reduced the voltage table in the program from 40 to 32 voltages. This was done because the bi-Gaussian waveform used on the USDA instrument has 40 voltages per cycle, while that for the USGS system uses only 32 voltages. The two approaches produce very similar results in terms of analytical sensitivity and signal-to-noise ratio for the several elements being determined. The difference in approach results from using different disc drives on the two computer systems, which necessitated different approaches to programming the system I/O.

The program CLKTST verified the function of the KW11-K real time clock (Digital Equipment Corporation, 1976c) which controls timing of the voltage outputs to provide for modulation at the desired frequency. The program listing is in Appendix 1c.

Modulation frequency must exceed the 50Hz frequency of the Xenon arc flicker component (Cochran and Hieftje, 1977; Harnly and O'Haver, 1981; O'Haver and others, 1978). For 56 Hz modulation, the bi-Gaussian waveform used for the USGS system requires that 896 voltages per second be output. This is achieved with a clock-issued interrupt every 1116 μsec to initiate the AA11-K output and simultaneous AD11-K conversions.

The clock is enabled (Digital Equipment Corporation 1976c) by setting bit 00 in the clock status register, and the clock count rate is set with bits 01-03 of the same register. The clock, once enabled at a specified frequency, counts clock ticks at that frequency from the initial count stored in the B counter register to the point where overflow of that register occurs, and then issues the interrupt. The register is 8 bits, and begins the count from zero (not one), filling at 255, and overflowing at 256. The starting count of the B counter register in conjunction with the clock rate, then, determines the modulation frequency. As just noted, 56Hz modulation with 32 voltage outputs per cycle requires an interrupt every 1116 μsec, or after 112 clock ticks at a clock counting rate of 100 KHz. The starting count in the B counter register must therefore be 256-112=140 (or 220 octal). The overflow, when it occurs, not only issues the interrupt, but also resets all necessary registers so that the count-down can begin again.

The first step in linking the several MACROS in the proper execution sequence was to combine the two programs AATEST and CLKTST in a program GAUS (Appendix 1d). Examination of the MVTABL: segments in the listings for AATEST and GAUS will identify the differences in voltage outputs for the USDA and USGS systems. This program enables approximately three minutes of continuous modulation under clock control without sampling of the ADC channels or storage of data on disc. It is most useful prior to the start of actual data collection for peaking the wavelength and for assuring that intensities in the absence of sample absorption are not saturating the 10V ADC upper limit for any of the active analytical channels.

Next, sampling of the ADC channels was added, using the logic of ADTEST, but omitting output of the conversions to the CRT. Such output occurs more slowly than the clock interrupts do, causing failure to receive and process all of them. Instead, the memory buffer for storage of the conversions was made as large as possible, and the data was examined after execution of the program by using the monitor DUMP command.

After this program modification, both the clock and conversion functions of the system were further tested by inputting a slow (6Hz) triangular waveform set for the full 10V output range of the ADC to one of the channels during program execution. When the clock interrupts are exactly timed and the conversions accurate, a dump of the memory buffer shows a very smooth rise and fall of the input voltage, with a constant delta voltage between ticks. Furthermore, holding the clock interrupt rate constant while changing the input waveform frequency to 3 or 12Hz should cause a halving or doubling of the delta voltage observed between ticks.

Then, a disc write of the memory buffer was added (WRITE.MAC, Appendix 1e) following the ADC conversions, but before the next clock tick, and the procedure of the preceding paragraph was repeated. Comparison of the data stored in the memory buffer with that written to disc assured that all collected data could be written to disc without loss or error before the next interrupt occurred. Editing to change the starting count of the B counter register for 70 Hz modulation and rerunning the test showed no change in ability of the disc write function to keep up accurately with the rate of data collection. No further variation in frequency of modulation to find the rate at which data would be lost by the write function was considered necessary.

Finally the DR11-K interrupt (Digital Equipment Corporation, 1975) (DR11.MAC, Appendix 1f) was inserted at the beginning of the combined program to trigger execution of all other functions. This resulted in a program, ACQGAU, which provided a one-time sequential execution of all SIMAAC control and data acquisition functions.

One-time execution of all control and data acquisition functions, however, is insufficient for a working atomic absorption system. It is also necessary that the acquired intensities be converted to absorbances and the data acquisition-manipulation be repeated for a series of standard and sample solutions. Because the computation of absorbances from intensities is quite slow in comparison to data acquisition, the final computation is done only for "active" channels, despite acquisition having been done for all 16 ADC channels. For each experiment, then, the operator must identify the active channels, and the total number of standards and samples to be measured, through an interactive start-up dialog.

The FORTRAN programs FLAME and FURN combine this start-up dialog with the individual control macros linked sequentially as just discussed, but rewritten as a callable subroutine (ACQSUB), and the FORTRAN subroutines which reduce the stored intensities to absorbances. These program listings appear with abbreviated flow diagrams in Appendix 2 (flame data acquisition) and Appendix 4 (furnace).

At this point a more detailed examination of the computation of absorbances from the raw intensity data is necessary. Recall that each voltage output to the galvanometer positions the refractor plate at a specific wavelength within the modulation interval of the analytical line, and that the transmitted intensity for that wavelength is obtained for each pass over the modulation interval. Intensities at the extremes of the modulation interval are used to establish I_0 while those at the line center determine I_1 for the absorbance which most closely approximates an AAL measurement for the given line. To obtain the best possible signal-to-noise ratio for this measurement, the refractor plate remains positioned at the line center for 12 clock ticks to establish I_1 and makes 4 closely spaced measurements at each extreme of the bidirectional pass across the interval for I_0. These sampling points are shown across the wavelength axis in Figure 2. Note that, except at the line center, the points differ for the forward and reverse direction half-cycle sweeps. This is also evident in the voltage table sections of the programs AATEST, AAGAUS, and ACQSUB which occur at label MVTBL.

Since, for flame data acquisition, the absorbance profile is a steady-state signal over the entire data collection period, the raw intensities at each wavelength can appropriately be averaged before proceeding to the calculation of absorbances. This reduces greatly the computational time (20 sec vs 2+ min), since only six absorbances per active channel rather than 6 per pass over the modulation interval per active channel are then necessary.

While the averaging on the USDA system is done in FORTRAN, for the USGS system it is done through a call to the MACRO subroutine AVGSUB. The USGS system lacks floating point hardware available on the USDA system, and is slower by roughly a factor of ten at performing multiplication and division. This forced a different approach to the computational scheme than that used for the USDA SIMAAC instrument.

The USDA system uses 260 unidirectional passes over the modulation interval, and ensemble averages them in groups of 10 before computing 26 sets of absorbances per channel per sample. This approach allows definition of the standard deviation of the absorbance signal for each of the 6 computations, for the very short, within sample, data collection time period. This is shot-noise limited, and reflects no effect from longer-term wavelength and order drift which can affect echelle system measurements if temperature changes occur over the course of analytical measurements. These within-sample standard deviations were used at USDA to determine the flame measurement detection limit for each calibration curve and to weight the results from the several

curves when concentrations were obtained for a sample from more than one of them (Harnly and O'Haver, 1981; Harnly and others, 1982; Miller-Ihli and Harnly, 1983).

Without floating point hardware, the computation time per sample becomes excessive when several absorbances based on group averaged intensities must be calculated, rather than calculate a single absorbance based on the grand average over the total data acquisition time. Furthermore, the averaging in FORTRAN requires more than 2 min/sample when floating point hardware is unavailable. To do the averaging in MACRO (5 sec/sample) by arithmetic shifts, the number of passes across the modulation interval must be evenly divisible by 8; the USGS system is therefore programmed for 512 unidirectional or 256 bidirectional passes, approximately 9.5 sec of data collection.

Wavelength and order drift of the polychromator is an unavoidable source of absorbance noise for the instrument, and it can be greater in magnitude than the within-sample absorbance noise. Therefore the flame detection limit as defined for the USGS instrument is based on the between-sample absorbance noise for multiple readings of the blank, rather than on within-sample noise. This eliminates the need to compute within-sample absorbance noise in the routine data collection program. The total reduction in execution time per sample resulting from MACRO averaging and elimination of multiple absorbance calculations approaches 4 minutes. Without this time reduction, the execution time per sample was so much greater than the 5-10 sec required by AAL as to eliminate the advantage of using a multielement system. Further, the very large per-sample timeframe made drift very much more pronounced than it otherwise would be, introducing unacceptable analytical error.

However, there is available on the USGS system a program, FLMDAT (Appendix 3), which provides within-sample standard deviations of absorbance. The program was run primarily to establish that the between-sample deviation is indeed larger (by a factor of 3-5) than the within-sample deviation, and that the programming approach taken is therefore valid. FLMDAT is a relatively simple modification of FLAME which uses the same MACRO averaging subroutine, but which then computes absorbances from intermediate group averages based on 32 bidirectional passes, rather than from the grand average of the 256 passes, as FLAME does.

The group averages are computed routinely in executing FLAME not because the values will be used in subsequent absorbance calculations, but primarily as a means of avoiding overflow error in the summation process for calculating the grand mean. Their use in absorbance calculations is the essential aspect of the modification of FLAME to FLMDAT. Execution time is about three times that for FLAME, still excessive for routine use, but considerably less than for the original approach which used FORTRAN averaging. In both FLAME and FLMDAT, the averaging is done as data acquisition is, for all channels, active or not. The averages are written to disk, filling one block as grand averages and eight blocks as group averages.

The intensities are collected in the order of voltage outputs (Figure 8a), beginning at approximately the middle of the modulation interval, sweeping to one extreme, reversing direction and sweeping to the other extreme, and finally reversing again and sweeping to the midpoint of the interval. This pattern of voltage output and data collection provides for smooth travel from the rest position and minimizes distortion of the waveform due to a lag in galvanometer response to the input voltage. For absorbance calculations, however, it is preferable to reorder the data so that each half cycle represents end point-to-end point travel across the modulation interval.

Once the FORTRAN main program has sorted the average intensities, it calls another subroutine CALSUB to perform the calculations for the series of absorbances which were previously defined in equation 1a.

The specific data points used for I_o and I_n for each of these absorbances are shown in Table IV. Note that all sets of data points are symmetrically distributed about the profile center. This provides for correction of sloping as well as uniform background absorption. Note as well that neither I_o nor I_n are truly monochromatic for any calibration curve since both are based on measurement at more than one refractor plate position. A third observation about these calculations is that other selections of points are possible, producing curves of different sensitivities, and the number of curves is by no means restricted to six. While the number of positions at which intensity measurements across the modulation interval can be made limits the ability to increase the number of curves above six, redundancy exists between curves, allowing a reduction in their number. With a change in the modulation waveform to one making repetitive measurements at fewer positions, reduction becomes necessary (Miller-Ihli and others, 1984b). Such a scheme has the advantage of reducing data processing time, and of improving the signal-noise ratio for the lower sensitivity absorbances which are computed.

Of the 6 calibration curves that result from these calculations, only curve 1 is useful at very low concentrations, because the absorbance profile has not yet broadened to the point that I_n $(n>1)$ differs from I_o. Eventually, however, the profile can broaden so much that I_o for the highly concentrated solution will indicate absorbance even at the profile endpoint, relative to the I_o measured for the blank or a low concentration solution. Figure 8b illustrates this for a series of Zn solutions.

The calculations made in the furnace data acquisition program differ from those discussed above because the furnace absorbance signal is a transient rather than a steady-state signal. This means that the averaging used in the flame program to reduce the computational time per sample cannot be used in the furnace program. Instead, the series of absorbances are computed for each pass across the modulation interval and then summed for peak area absorbance and treated by a routine to determine peak absorbance.

TABLE IV

Flame atomization

Measurement positions used for the calculation of absorbances on the successive calibration curves

Curve	Points Used* for I_n	Points Used* for I_o
1	5-12 21-28	1-4 and 13-16 17-20 and 29-32
2	5,12,21,28	1,16,17,32
3	4,13,20,29	1,16,17,32
4	3,14,19,30	1,16,17,32
5	2,15,18,31	1,16,17,32
6	1 and 17	16 and 32

* Points 1-16 represent those for travel in one direction after the sorting is done for computational purposes, and points 17-32 are those for travel in the reverse direction across the modulation interval.

To avoid excessive computational time, only three absorbances are calculated, using the points shown in Table V. While the time required for these calculations greatly exceeds that for the flame program, it is approximately comparable to the time requirements of the furnace dry-char-atomization-cooldown sequence, and therefore not a concern. The computation time required by AAL furnace instruments with computer data stations, for example the PE5000 Zeeman with Data Station 360, is as long or longer for a single element, depending on the particular program being run.

Reduction of the number of absorbances to three does not limit the useful extension of the calibration range. In the first place, some overlap in the useable ranges of the six curves developed from flame calculations has already been noted. Judicious selection of those for elimination simply removes the redundancy. Additionally, at very high concentrations in the furnace, there is considerable carryover contamination from one sample to the next atomized, especially for the more refractory elements (Harnly and others, 1984). The carryover contamination is due to condensation of the analyte on the cooler ends of the tube and on the cones or to retention in the graphite pore spaces of some of the analyte after the completion of a sample atomization cycle. Full use of the extended calibration range is therefore subject to serious analytical error. Loss of the upper end of that range, therefore, by elimination of the least sensitive calibration curves, is not a problem.

Further documentation of the system software discussed in this report can be found in the comment lines of the program codes themselves, appendices 1-4.

The programs required for examination or plotting of the absorbance data collected using FLAME, FLMDAT, and FURN, and for computation of concentrations from the absorbances will be the subject of another report. A procedures manual for daily operation of the instrument and routine use of all software associated with it will also appear separately.

TABLE V

Furnace Atomization

Measurement positions used for the calculation of absorbances of the successive calibration curves

Curve	Positions used for I_n	Positions Used for I_o
1	5-12 21-28	1-4 and 13-16 17-20 and 29-32
2	5,12,21,28	1,16,17,32
3	4,13,20,29	1,16,17,32

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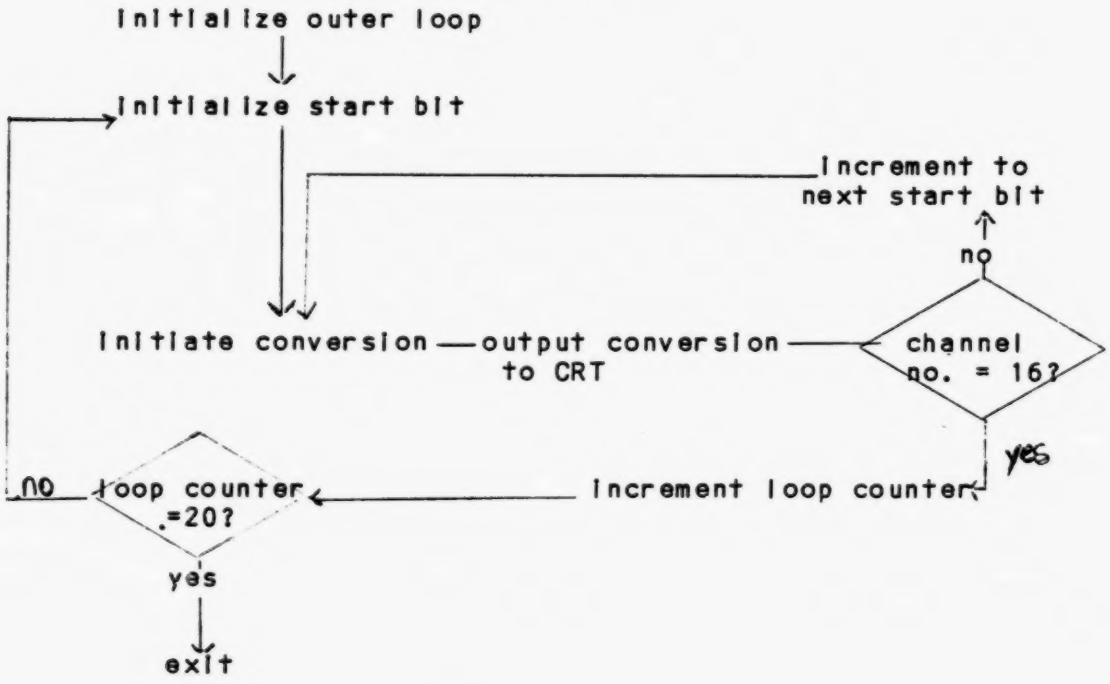
```
        .TITLE ADTEST
        .MCALL  .EXIT,.TWAIT,.TTYOUT,.PRINT
;TRIGGER A CONVERSION ON EACH OF 16 A/D CHANNELS AND OUTPUT
;THE CONVERSIONS IN 132 COLUMN FORMAT IN OCTAL ON THE CRT.
;LOOP THROUGH ALL CHANNELS AND OUTPUT 20 TIMES
ADSR=170400
ADBR=170402
LCV:    .WORD   20.
NOCHAN: .WORD   16.
STRTBT: .WORD   1
START:  MOV     LCV,R3          ;INITIALIZE LOOP FOR 20 CYCLES
START1: MOV     NOCHAN,R2       ;  AND CHANNEL NO. FOR INNER LOOP
        MOV     STRTBT,R1       ;INITIALIZE START BIT FOR AD11-K CHANNELS
        CLR     @#ADSR          ;  AND CLEAR AD11-K STATUS REGISTER
LOOP:   MOV     R1,@#ADSR       ;SET START BIT
WAIT:   TSTB    @#ADSR          ;  AND TEST FOR DONE FLAG,
        BPL     WAIT            ;  LOOPING IF CONVERSION NOT DONE
        MOV     @#ADBR,R0       ;  AND MOVING DATA TO R0 IF DONE
        JSR     PC,OUTOCT       ;JUMP TO OUTPUT SUBROUTINE, DATA OUT AT CRT
        ADD     #400,R1         ;INCREMENT START BIT TO NEXT CHANNEL
        SOB     R2,LOOP         ;  AND LOOP TO NEXT CHANNEL
        .TTYOUT #15             ;INNER LOOP ALL CHANNELS COMPLETE
        .TTYOUT #12             ;  SO OUTPUT <LF><CR>
        .TWAIT  #AREA,#TIME     ;WAIT AND THEN REPEAT
        SOB     R3,START1       ;  OUTER LOOP 20 CYCLES THROUGH ALL CHANNELS
        .EXIT
AREA:   .WORD   0,0
TIME:   .WORD   0,20
        .END    START
;       END ADTEST MAIN PROGRAM
;       BEGIN OUTPUT SUBROUTINE
OUTOCT:
        MOV     R0,-(SP)
        MOV     R1,-(SP)
        MOV     R2,-(SP)
        MOV     R3,-(SP)
        MOV     R4,-(SP)        ;SAVE REGISTERS USED IN MAIN
        MOV     #PV,R1          ;INITIALIZE PLACE VALUE
        MOV     #5,R2           ;INITIALIZE LOOP FOR NO. OF DIGITS
        MOV     #VAL,R3         ;INITIALIZE OUTPUT POINTER
NEXT:   MOV     #-1,R4          ;INITIALIZE DIGIT VALUE TOP 177777
COUNT:  INC     R4              ;UPDATE DIGIT VALUE
        SUB     (R1),R0         ;SUBTRACT PLACE VALUE FROM DATA VALUE
        BHIS    COUNT           ;  UNTIL OVERSUBTRACTED
        ADD     (R1)+,R0        ;CORRECT FOR OVERSUBTRACTION
        ADD     #60,R4          ;CONVERT DIGIT TO ASCII
        MOVB    R4,(R3)+        ;PUT ASCII DIGIT IN OUTPUT ARRAY
        SOB     R2,NEXT         ;REPEAT FOR NEXT DIGIT
        .PRINT #VAL             ;ALL DIGITS IN ARRAY-.PRINT IT
        MOV     (SP)+,R4
        MOV     (SP)+,R3
        MOV     (SP)+,R2
        MOV     (SP)+,R1
        MOV     (SP)+,R0        ;RESTORE ALL REGISTERS
        RTS     PC              ;AND RETURN TO CALLING PROGRAM
PV:     .WORD   10000,1000,100,10,1     ;PLACE VALUES
VAL:    .BLKB   5                       ;ALLOCATE OUTPUT ARRAY SPACE
        .BYTE   0
        .EVEN
;END OF SUBROUTINE
        .END START
```

ADTEST Flow Diagram



AA11-K START/STOP BIT TABLE

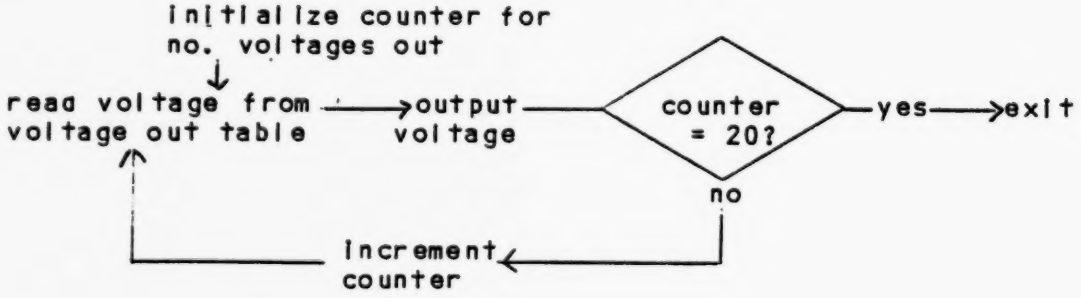
channel*	start bit	stop bit
0	001	200
1	401	600
2	1001	1200
3	1401	1600
4	2001	2200
.....		
.....		
.....		
12	6001	6200
13	6401	6600
14	7001	7200
15	7401	7600

* channel numbering in octal, beginning with 0, to correspond to programming requirements.

APPENDIX 1B

```
        .TITLE  AATEST
        .MCALL  .EXIT,.TWAIT
        .IDENT  /AATEST/
DACODR=170420
NOVLT:  .WORD   20
START:  MOV     NOVLT,R4
        MOV     #VOLT,R3
START1: MOV     (R3)+,@##DACODR
        .TWAIT  #AREA,#TIME
        SOB     R4,START1
        .EXIT
VOLT:   .WORD   7600,7200,6600,6200,5600,5200
        .WORD   4800,4200,3600,3200,2600,2000
        .WORD   1600,1200,600,200
AREA:   .WORD   0,0
TIME:   .WORD   0,60
        .END    START
```

AATEST Flow Diagram



APPENDIX IC

```
        .TITLE CLKTST.MAC
;       THIS PROGRAM TESTS THE KW11-A REAL TIME CLOCK.
;       THE CLOCK B IS SET TO GENERATE AN INTERRUPT EVERY SECOND
;       WHICH IS SERVICED TO CTRL-G (RING BELL) AT THE TERMINAL
;
        .MCALL .TTOUT
;
        RATE    =       1.      ;SET CLOCK RATE AT 100 HZ
        INTOV   =       100     ;ENABLE INTERRUPT ON OVERFLOW
        GOBIT   =       1
        CBSR    =       177432  ;STATUS REGISTER ADDRESS
        CBBR    =       177434  ;CLOCK B BUFFER REGISTER ADDRESS
        CBIV    =       364     ;CLOCK B INTERRUPT VECTOR

CLKSET: MOV     #CLKINT,@#CBIV  ;PUT ADDRESS OF INTERRUPT SERVICE
                                ;ROUTINE IN INTERRUPT VECTOR
        MOV     #340,@#CBIV+2   ;SET PRIORITY TO 7
        BIS     #RATE,@#CBSR    ;SET RATE IN STATUS REGISTER
        BIS     #INTOV,@#CBSR   ;ENABLE INTERRUPT
        MOV     #200,@#CBBR     ;SET DOWNCOUNTER 100
        BIS     #GOBIT,@#CBSR   ;START CLOCK

LOOP:   NOP
        BR      LOOP

CLKINT: .TTOUT  #7              ;RING BELL
        RTI

        .END CLKTST
```

```
        .TITLE PROGRAM FOR AA11 TEST WITHOUT ANY A-D CONVERSIONS
        .MCALL .EXIT
        .IDENT  /GAUS/
;THIS IS AN EDIT OF AATEST WHICH ADDS A CLOCK FEATURE TO ENABLE
;APPROX. THREE MIN. OF WAVELENGTH MODULATION AT 56 CYCLES PER SECOND
;(IE 56 UNIDIRECTIONAL PASSES/SEC OVER THE MODULATION INTERVAL)
;THE CLOCK INTERRUPTS AT 16 TIMES THAT RATE IN ORDER THAT EACH
;VOLTAGE OUTPUT ACROSS THE INTERVAL BE GENERATED BY THE INTERRUPT
DACODR=170420
CLKBCT=220
CBSR=170432
CBBR=170434
CBIV=364
NOCYCL: .WORD   5000.
MVINDX: .WORD   -62.
;
;PROGRAM SETS UP CLOCK AND TIMES COUNTING INTERRUPTS UNTIL FULL
;  MODULATION TIME INTERVAL HAS ELAPSED, THEN EXITS
;
START:  MOV     #4000,@#DACODR          ;INIT DAC OUTPUT AT ZERO VOLTS
        MOV     #CLKBCT,@#CBBR          ;890 MICROSEC. BETW INTERRUPTS
        MOV     #CLKINT,@#CBIV          ;MOV SERVICE ROUTINE ADDR TO
                                        ;  INTERRUPT VECTOR ADDRESS
        MOV     #340,@#CBIV+2           ;SET PRIORITY FOR INTERRUPT
        MOV     #105,@#CBSR             ;ENABLE CLOCK B INTERRUPT
IDLE:   CMP     NOCYCL,#0               ;TEST -  LAST CYCLE COMPLETED?
        BEQ     ENDO                    ;  AND EXIT IF YES
        BR      IDLE                    ;    IF NOT WAIT FOR NEXT INTERRUPT
                                        ;    REPEATEDLY TIL LAST CYCLE DONE
;
; INTERRUPT SERVICE ROUTINE
;
CLKINT: MOV     R0,-(SP)
        MOV     R1,-(SP)                ;SAVE REGISTERS
        MOV     R2,-(SP)
        MOVB    MVINDX,R2               ;INITIALIZE VOLTAGE INDEX
        MOV     VOLT+64.(R2),@#DACODR   ; AND MOVE VOLTAGE TO AA BUFFER
        ADD     #2,R2                   ;INCREMENT INDEX
        BLT     CLK010                  ; AND BRANCH IF INDEX DOES NOT
                                        ;   NEED RESETTING, ELSE
        MOV     #-64.,R2                ;RESET INDEX FOR NEXT CYCLE
        DEC     NOCYCL                  ;  AND DECREMENT CYCLE COUNTER
CLK010: MOVB    R2,MVINDX               ;SAVE VOLTAGE TABLE INDEX
                                        ;  FOR NEXT INDIVID. VOLT OUT
        MOV     (SP)+,R2                ;RESTORE REGISTERS
        MOV     (SP)+,R1
        MOV     (SP)+,R2
        MOV     #105,@#CBSR             ;  AND RESTORE START CLOCK
CLK020: RTI                             ;RETURN FROM INTERRUPT
ENDO:   CLR     @#CBSR                  ;STOP B CLOCK
        .EXIT                           ;AND EXIT PROGRAM EXECUTION
;
;MODULATION VOLTAGE TABLE
;
VOLT:   .WORD   3237,3547,4000,4000,4000
        .WORD   4000,4000,4000,6203,7173
        .WORD   7526,7666,7777,5670,5214
        .WORD   4704,4540,4230,4000,4000
        .WORD   4000,4000,4000,4000,1575
        .WORD   0605,0251,0112,0000,1267
        .WORD   2063,3075
        .END    START
```

APPENDIX IE

```
        .TITLE WRITE.MAC
        .MCALL .EXIT,.PRINT,.ENTER,.WRITE,.CLOSE
        .IDENT  /WRITE/
;
;THIS IS AN EXIT OF GAUS WHICH ADDS ADC CONVERSIONS BETWEEN
;CLOCK INTERRUPTS, WRITING THE CONVERSIONS FOR EACH CHANNEL TO DISC
;
DACODR=170420
CLKBCT=220
CBSR=170432
CBBR=170434
CBIV=364
NOCYCL: .WORD   200.
MVINDX: .WORD   -62.
;
;PROGRAM SETS UP CLOCK AND IDLES UNTIL INTERRUPT OCCURS
;THEN OUTPUTS A VOLTAGE TO SCANNER AND MAKES ADC CONV. ALL CHAN
;WRITING THE CONVERSIONS TO MEMORY BUFFER;
;ADDS OCCURRENCE TO INTERRUPT COUNTER AND CYCLES
;UNTIL MODULATION TIME INTERVAL HAS ELAPSED,
;THEN WRITES BUFFER TO DISK AND EXITS
;
;INITIALIZE AD VARIABLES, ALLOCATE MEMORY SPACE
;
ADSR=170400
ADBR=170402
STRBT=1
NOCHAN= 16
BUFFER: .BLKW   16.*200.
FILSIZ=200
;
;PREPARE FOR WRITE
;
CNT:    .BLKW   6
FILSPC: .RAD 50 /DL1/                   ;NAME FILE FOR WRITE
        .RAD 50 /ADCONV/
        .RAD 50 /DAT/
FE:     .ASCIZ "ENTER FAILED"<12><15>   ;ERROR MESSAGES
FW:     .ASCIZ "WRITE FAILED"<12><15>
DONE:   .ASCIZ "WRITE SUCCESSFUL"<12><15>       ;SUCCESS MESSAGE
        .EVEN
;
;SET UP CLOCK
;
START:  MOV     #4000,@#DACODR          ;INIT DAC OUTPUT AT ZERO VOLTS
        MOV     #CLKBCT,@#CBBR          ;890 MICROSEC. BETW INTERRUPTS
        MOV     #CLKINT,@#CBIV          ;MOV SERVICE ROUTINE ADDR TO
                                        ;  INTERRUPT VECTOR ADDRESS
        MOV     #340,@#CBIV+2           ;SET PRIORITY FOR INTERRUPT
        MOV     #105,@#CBSR             ;ENABLE CLOCK B INTERRUPT
IDLE:   CMP     NOCYCL,#0               ;TEST -  LAST CYCLE COMPLETED?
        BEQ     END0                    ;  AND EXIT IF YES
        BR      IDLE                    ;    IF NOT WAIT FOR NEXT INTERRUPT
                                        ;    REPEATEDLY TIL LAST CYCLE DONE
;
; INTERRUPT SERVICE ROUTINE
; OUTPUTS VOLTAGE AND PERFORMS ADC CONVERSIONS
;
CLKINT: MOV     R0,-(SP)
        MOV     R1,-(SP)                ;SAVE REGISTERS
        MOV     R2,-(SP)
        MOV     R3,-(SP)
        MOV     #NOCHAN,R1              ;INITIALIZE CHANNEL COUNTER
        MOV     #BUFFER,R3              ;  AND BUFFER ADDRESS
```

```
        CLR     @#ADSR                  ;CLEAR AD STATUS REGISTER
LOOP:   INC     @#ADSR                  ;BEGIN AD CONVERSIONS
WAIT1:  TSTB    @ADSR                   ;  AND SEE IF DONE
        BPL     WAIT1                   ;IF NOT WAIT, ELSE
        MOV     @#ADBR,(R3)+            ;  MOVE DATA TO BUFFER
        ADD     #400,@#ADSR             ;  & INCR START BIT TO NEXT CH
        SOB     R2,LOOP                 ;REPEAT UNTIL ALL CHANNELS DONE
        MOVB    MVINDX,R2               ;INITIALIZE VOLTAGE INDEX
        MOV     VOLT+64.(R2),@#DACDBR   ;  AND MOVE VOLTAGE TO AA BUFFER
        ADD     #2,R2                   ;INCREMENT INDEX
        BLT     CLK010                  ;  AND BRANCH IF INDEX DOES NOT
                                        ;    NEED RESETTING, ELSE
        MOV     #-64.,R2                ;RESET INDEX FOR NEXT CYCLE
        DEC     NOCYCL                  ;  AND DECREMENT CYCLE COUNTER
CLK010: MOVB    R2,MVINDX               ;SAVE VOLTAGE TABLE INDEX
                                        ;  FOR NEXT INDIVID. VOLT OUT
        MOV     (SP)+,R2                ;RESTORE REGISTERS
        MOV     (SP)+,R1
        MOV     (SP)+,R2
        MOV     #105,@#CBSR             ;  AND RESTORE START CLOCK
CLK020: RTI                             ;RETURN FROM INTERRUPT
;
;ALL INTERRUPTS HAVE BEEN PROCESSED: STOP CLOCK AND WRITE TO DISK
;
END0:   CLR     @#CISR                  ;STOP M CLOCK
WRTSET: .ENTER  #EMT,#3,#FILSPC,#FILSIZ ;OPEN FILE
        BCC     FAILE                   ;BRANCH IF ENTER FAILS, ELSE
        .WRITE  #EMT,#3,#BUFFER#,200.   ; WRITE FULL BUFFER TO DISK
        BCS     FAILW                   ;BRANCH IF WRITE FAILS, ELSE
        .CLOSE  #3                      ; CLOSE FILE AND
        .PRINT  #DONE                   ; PRINT WRITE SUCCESSFUL MESSAGE
        BR END                          ;AND EXIT PROGRAM EXECUTION
FAILE:  .PRINT  #FE
        BR END
FAILW:  .PRINT #FW
END:    .EXIT
;
;MODULATION VOLTAGE TABLE
;
VOLT:   .WORD   3237,3547,4000,4000,4000
        .WORD   4000,4000,4000,6203,7173
        .WORD   7526,7666,7777,5670,5214
        .WORD   4704,4540,4230,4000,4000
        .WORD   4000,4000,4000,4000,1575
        .WORD   0605,0251,0112,0000,1267
        .WORD   2063,3075
        .END    START
```

APPENDIX IF

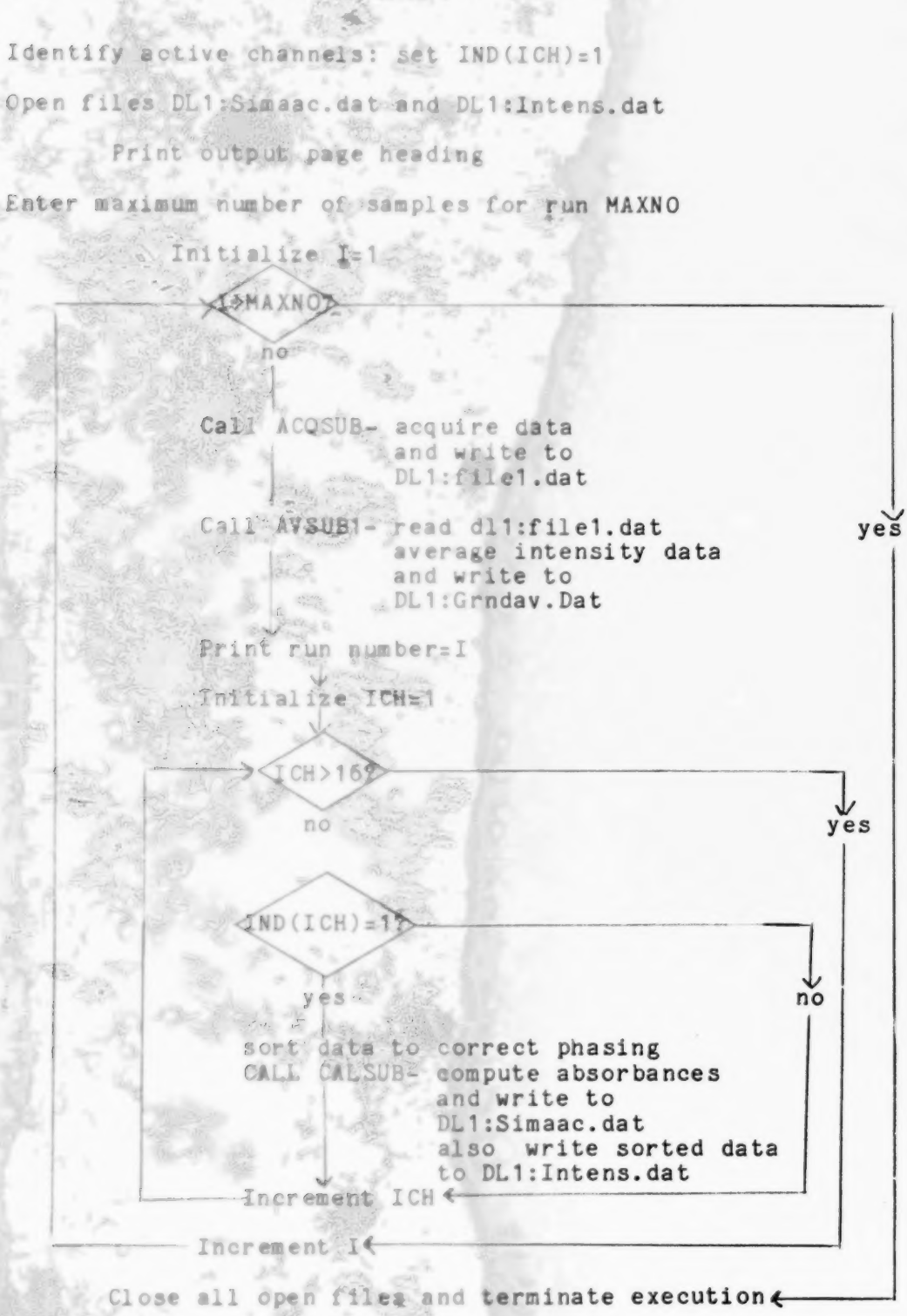
```
        .TITLE DRII
        .MCALL .PRINT .EXIT .TWAIT

; THIS PROGRAM WAITS IN A TIGHT LOOP AND WHEN INTERRUPTED, EXECUTES AN
; INTERRUPT SERVICE ROUTINE
; THE INTERRUPT IS GENERATED WHEN PIN A OF J1 I/O PORT GOES HIGH
; THE SERVICE ROUTINE IMMEDIATELY DISABLES THE INTERRUPT AND CONTINUES
; IN THE WAIT LOOP, MAKING THE INTERRUPT A ONE SHOT DEAL
;
;
        DRCSR   =       167770  ;CSR FOR DRV11
        DINTV   =       300     ;INTERRUPT VECTOR A
        INTENB  =       100     ;INTERRUPT A ENABLE
        INTGEN  =       200     ;INTERRUPT A GENERATE
;
;
START:  MOV     #DINTV,R1               ;R1=INTERRUPT VECTOR ADDRESS
        MOV     #INTSER,(R1)            ;LOAD SERVICE ROUTINE VECTOR
        BIS     #INTENB,@#DRCSR         ;ENABLE INTERRUPT A
LOOP:   NOP
        .PRINT  #WAIT                   ;WAITING MESSAGE
        .TWAIT  #AREA,#TIME             ;WAIT 1 SEC
        BR      LOOP                    ;LOOP AGAIN
        .EXIT

INTSER: .PRINT  #SUCESS                 ;PRINT SUCESS MESSAGE
        BIC     #INTENB,@#DRCSR         ;DISABLE INTERRUPT A
        RTI
        .EXIT

AREA:   .WORD   0,0
TIME:   .WORD   0,60.                   ;1 SEC AT 60 HZ

WAIT:   .ASCIZ  "I'M PATIENTLY WAITING"<12><15>

SUCESS: .ASCIZ  "PROGRAM WAS INTERRUPTED, AND THIS IS THE RESULT"<12><15><7>
        .EVEN
        .END    START
```

APPENDIX 2

```
PROGRAM ILAB
C
C       THIS PROGRAM (ILAB) CALLS ACQSUB TO COLLECT THE DATA WHICH
C       CONSTITUTES DL1:[1,1]IL1.DAT
C       THEN CALLS AVGSUB WHICH READS THAT FILE AND AVERAGES IT
C       NEXT REQUIRES DATA FOR ABSORBANCE CALCULATIONS
C       CALLS CALSUB TO PERFORM THE ABSORBANCE CALCULATIONS
C       THEN LOGS THE (NORMALIZED) INTENSITY DATA IN DL1:INTENS.DAT
C       AND THE CALCULATED ABSORBANCES IN DL1:SMAAC.DAT
C       AND LOOPS FOR NEXT SAMPLE OR A MAXIMUM DEFINED BY MAXRUN
C
        DIMENSION IDATA(512),IBUF(16,32),INP(16)                    <-- C
        REAL ABS(8)                                                 C LINK WITH ACQSUB, AVGSUB, CALCAB,
        EQUIVALENCE (IDATA(1), IBUF(1))                             C                  SYSLIB, FORLIB
        COMMON /BUFS/ IBUF,ABS
        INTEGER ACNT,IBUF(32)
        BYTE EL(32)
        DATA EL(1),EL(2),EL(3),EL(4)/1HI,1HF,1HZ,1HN/
        DATA EL(5),EL(6),EL(7),EL(8)/1HE,1HD,1HS,1HR/
        DATA EL(9),EL(10),EL(11),EL(12)/1HB,1HI,1HR,1HF/
        DATA EL(13),EL(14),EL(15),EL(16)/1HC,1HO,1HM,1HI/
        DATA EL(17),EL(18),EL(19),EL(20)/1HL,1HK,1HS,1HN/
        DATA EL(21),EL(22),EL(23),EL(24)/1HC,1HO,1H ,1HV/
        DATA EL(25),EL(26),EL(27),EL(28)/1HM,1HN,1HA,1HD/
        DATA EL(29),EL(30),EL(31),EL(32)/1HF,1HR,1HN,1HI/
C
C       SET UP ACTIVE CHANNELS AND SELECT MONITOR CHANNEL-DEFAULT TO
C
        DO 2 I=1,16
                IND(I)=1
                TYPE *,' IS CHANNEL ',I,' ACTIVE?'
                ACCEPT 1499,YESNO
                IF (YESNO .EQ. 'N')IND(I)=0
2       CONTINUE
        IF (IND(11) .EQ. 1)IMON=11
3       TYPE *,' MONITOR CHANNEL OTHER THAN 11?'
        ACCEPT 1499, YESNO
        IF (YESNO .NE. 'Y' .AND. YESNO .NE. 'N')GO TO 3
        IF (YESNO .EQ. 'Y')TYPE *,'ENTER NO. FOR MONITOR CHANNEL'
        IF (YESNO .EQ. 'Y')ACCEPT 1504,IMON
C
C
        TYPE *,' ENTER MAXIMUM NO. SAMPLES FOR DATA COLLECTION RUN'
        ACCEPT *,MAXRUN
C
        OPEN (UNIT=15,TYPE='NEW',ACCESS='DIRECT',NAME='DL1:SMAAC.DAT',
     1    RECORDSIZE=8,INITIALSIZE=100)
        OPEN (UNIT=16,TYPE='NEW',ACCESS='DIRECT',NAME='DL1:INTENS.DAT',
     1     RECORDSIZE=16,INITIALSIZE=100)
C       DL1:SMAAC.DAT RECORD IS 8 ABSORBANCES AS REAL DATA SO RECSIZ=8
C       DL1:INTENS.DAT RECORD IS 32 INTENSITIES AS INTEGERS SO RECSIZ=16
C
        PRINT 1500
        PRINT 1501
C
        RCNT=1
        DO 1000 NA=1,MAXRUN
                TYPE *,'READY FOR TRIGGER'
                CALL ACQSUB
C               TYPE *,' DATA ACQUIRED, WRITTEN TO DISK'
                CALL AVGSUB
C               TYPE *,'AVERAGES COMPUTED, WRITTEN TO DISK'
                OPEN (UNIT=3,TYPE='OLD',ACCESS='DIRECT',NAME='DL1:GRNDAV.DAT',
     1            RECORDSIZE=256)
C       DL1:GRNDAV.DAT RECORD IS 512 INTENSITIES AS INTEGERS SO RECSIZ=256
```

```
C
C       VOLTAGE INDEX=1 AT A MIDPOINT IN THE MODULATION INTERVAL
C       RESULTING IN DATA ORDER IN DI1:GRNDAV.DAT WHICH IS AWKWARD
C       FOR USE IN ABSORBANCE CALCULATION SUBROUTINE
C       DO 5 AND DO 6 REORDER THE DATA SO THAT IBUF(1) TO IBUF(16)
C       REPRESENT INTENSITY DATA FOR PASS FROM LOWEST TO HIGHEST WAVELENGTH
C       IN THE MODULATION INTERVAL AND IBUF(17) TO IBUF(32) REPRESENT
C       DATA FOR REVERSE DIRECTION PASS
C
              PRINT 1502,KK
              READ (3 '1)(IDATA(I),I=1,512)
                    DO 10,ICH=1,16
                          IF (IND(ICH) .EQ. 0) GO TO 10
                          DO 5,IPOS=1,14
                                JJ=IPOS+18
                                IBUF(JJ)=IBUF(ICH,IPOS)
5                         CONTINUE
                          DO 6,IPOS=15,32
                                JJ=IPOS-14
                                IBUF(JJ)=IBUF(ICH,IPOS)
6                         CONTINUE
                    CALL CALSUB
                          J=ICH*2
                          IF (ICH .EQ. IMON)TYPE 1505,KK,(ABS(I),I=1,6)
                          PRINT 1503,((EL(K),K=J-1,J),(ABS(I),I=1,6))
                          WRITE (15 'RCNT) (ABS(I),I=1,6)
                          WRITE (16 'RCNT) (IBUF(JJ),JJ=1,32)
                          RCNT=RCNT+1
10                  CONTINUE
              CLOSE (UNIT=3)
1000    CONTINUE
        CLOSE (UNIT=15)
        CLOSE (UNIT=16)
C
1499    FORMAT (A1)
1500    FORMAT (/139,'SIMAAC ANALYSES: CALCULATED ABSORBANCES')
1501    FORMAT (//6X,'EL ',2X,'ABS(1)',7X,'ABS(2)',7X,
     1    'ABS(3)',7X,'ABS(4)',7X,'ABS(5)',7X,'ABS(6)')
1502    FORMAT (/3X,'RUN ',I2)
1503    FORMAT (6X,2A1,5X,6(F7.4,5X))
1504    FORMAT (I2)
1505    FORMAT (3X,'RUN ',I2,3X,6(F7.4,2X))
        STOP
        END
```

ABBREVIATED FLOW DIAGRAM: PROGRAM FLAME



```
RATE    =       220             ;SET COUNTER TO 1KHZ
;COUNTER IS COUNTED UP FROM INITIAL VALUE IN B REGISTER TO 256, WHEREUPON
;CLOCK B COUNTER OVERFLOWS AND INTERRUPT IS GENERATED.  WITH INITIAL
;VALUE OF 220 AND COUNTING RATE 100 KHZ, A MODULATION FREQUENCY OF 56HZ
;IS ACHIEVED.

                .TITLE ACQSUB           ;DERIVES FROM MDACQ1
        .GLOBL ACQSUB
;
;       WRITTEN 7-1-86 AS CALLABLE SUBROUTINE CALLED FROM
;       FLAME, FLMDAT, OR FORN FOR SIMAAC INSTRUMENT CONTROL
;       AND DATA ACQUISITION
;


;BASED IN PART ON MDACQ1 WRITTEN BY DOUGLAS SEWARD, USDA, 3-4-85
;ACQGAU A STANDALONE PROGRAM VERSION OF THE SUBROUTINE
;A COMPOSITE OF AATEST,ADTEST,CLKIST,DR11,WRITE
;FOR SIMAAC WITH MODIFICATIONS 5-86 BY JSK FOR USGS SYSTEM SPECS
;DATA ACQUISITION AND MODULATION WAVEFORM CONTROL
;MODIFIED 16-JUN-87 TO HAVE MESSAGES SENT FROM MAIN NOT SUBROUTINE
;  BY SIMPLY CONVERTING ALL PRINT MESSAGE COMMANDS TO COMMENT LINES
;
;       THIS PROG SETS UP DATA ACQ FOR TRIGGERING BY DR11 INTERRUPT
;       THIS PROGRAM OUTPUTS A VOLTAGE FROM THE WAVEFORM TABLE AND THEN
;       TAKES DATA FROM THE ADC DURING AN INTERRUPT SERVICE ROUTINE
;       ENTERED THROUGH A CLOCK GEN INTERR AND WRITES THE DATA TO DISK.
;
;       EDITED 6-11-86 TO BIGAUSSIAN VOLTAGE TABLE AND NO. BLOCKS NEEDED
;       FOR WRTAV.MAC TO REDUCE FIRST TO 8 GROUP AVERAGES AND THEN TO
;       A SINGLE GRAND AVERAGE INTENSITY/CHANNEL/VOLT
;
        .MCALL  .MTPS, .TTYOUT, .PRINT .SRESET
        .MCALL   .FETCH, .ENTER, .WRITE,.CLOSE
;       .LIST TTM
.SBTTL  BUFFER
;.PSECT DATA
;*********************BUFFER DATA*********************************************
;                                                                            *
;                                                                            *
;                                                                           ***
;                                                                            *
;FILSIZ IS PRESET DURING ASSEMBLY, TO THE TOTAL NO. BLOCKS
;REQUIRED TO STORE DATA FROM 16 CHANNELS, ONE SAMPLE , 256 UNIDIRECTIONAL
;PASSES ACROSS THE MODULATION WAVEFORM, WHICH IS 9 SEC OF DATA ACQUISITION
;
;BUFSIZ IS SIZE OF BUFFER FOR A SINGLE DISK WRITE; MUST BE EVENLY DIVISIBLE
;BY EIGHT AND EVENLY DIVISIBLE INTO FILSIZ-- REQUIREMENT BASED IN PART ON
;AVERAGING ROUTINE USED SUBSEQUENTLY IN CALLING MAIN
;
;
FILSIZ  ==      512.            ;NUMBER OF BLOCKS IN FILE
BUFSIZ  ==      16.             ;NUMBER OF BLOCKS IN BUFFER
WRDCNT  ==      16.*256.        ;WORD COUNT OF BUFFER
BUFF0:  .BLKW   BUFSIZ*400      ;192*16 CONVERSIONS (12 BLOCKS)
BUFF1:  .BLKW   BUFSIZ*400      ;DITTO
JUNK:   .BLKW   10              ;BUFFER OVERRUN SPACE
BF0ADR: .WORD   0               ;START ADDRESS OF BUFFER 0
BF0END: .WORD   0               ;END ADDR OF BUFFER 0
BF1ADR: .WORD   0               ;START ADDRESSOF BUFFER
BF1END: .WORD   0               ;END ADDR OF BUFFER 1
CUREND: .WORD   0               ;END ADDR OF CURRENT BUFFER
CURBUF: .WORD   0               ;START ADDR OF CURRENT BUFFER
WRTBFR: .WORD   0               ;START ADDR OF BUFFER TO BE WRITTEN
POINTR: .WORD   0               ;POINTS TO NEXT AVAIL ADDR IN BUFFER
```

```
BUFIND: .BYTE   0               ;BUFFER INDICATER
BFRFUL: .BYTE   0               ;BUFFER FULL FLAG
        .EVEN
;                                                                              *
;                                                                             ***
;                                                                              *
;                                                                              *
;*******************************************************************************
;.PSECT CODE
;       THIS SECTION OF CODE INITIALIZES THE BUFFER VARIABLES

ACQSUB: MOV     #BUFF0,BF0ADR           ;SAVE START ADDRESS OF BUFF0
        MOV     #BUFF1,BF1ADR           ;SAVE START ADDRESS OF BUFF1
        MOV     #BUFF1-2,BF0END         ;SET BUFFER 0 END
        MOV     #JUNK-2,BF1END          ;SET BUFFER 1 END
        MOV     BF0END,CUREND           ;CURRENT END OF BUFFER =BF0END
        MOV     #BUFF0,POINTR           ;INITIALIZE BUFFER POINTER
        MOV     #BUFF0,CURBUF           ;INIT ADDR OF CURRENT BUFFER
        MOVB    #0,BUFIND               ;INIT BUFFER INDICATOR
        MOVB    #0,BFRFUL               ;INIT BUFFER FULL FLAG
        MOV     #0,BLKCTR               ;INIT BLOCK COUNTER
        BR      WRTSET          ;GO ON TO WRITE SET UP

.SBTTL WRITE
;.PSECT DATA

;*****************************WRITE ROUTINE DATA*********************************
;                                                                              *
;                                                                              *
;                                                                             ***
;                                                                              *
EMT:    .BLKW   6       ;6 WORD EMT BLOCK
BLKCTR: .WORD   0               ;BLOCK COUNTER
FILSPC: .RAD50  /DL1/
        .RAD50  /FILE1/
        .RAD50  /DAT/   ;FILE DESCRIPTOR
        .EVEN
FF:     .ASCIZ "FETCH FAILED"<12><15>
FE:     .ASCIZ "ENTER FAILED"<12><15>
FW:     .ASCIZ "WRITE FAILED"<12><15>
DONE:   .ASCIZ "WRITE SUCESSFUL"<12><15>
        .EVEN
;                                                                              *
;                                                                             ***
;                                                                              *
;                                                                              *
;*******************************************************************************

;.PSECT CODE
;THIS SECTION OF CODE GETS THE HANDLER (.FETCH), ALLOCATES SPACE
;ON THE DEVICE, AND RETURNS CONTROL TO THE MAIN PROGRAM

WRTSET: .FETCH  @#50,#FILSPC                    ;GET DEVICE HANDLER
        BCS     FAILF                           ;BR IF FAILED TO GET HANDLER
        .ENTER  #EMT,#3,#FILSPC,#FILSIZ         ;ALLOCATE SPACE ON DEVICE
        BCS     FAILE                           ;BR IF ENTER FAILED
        BR      CLKSET          ;GO ON TO SET-UP CLOCK

FAILE:  .PRINT  #FE             ;PRINT / ENTRY FAILED /
        RTS     PC

FAILF:  .PRINT  #FF             ;PRINT / FETCH FAILED /
        RTS     PC
        .SBTTL  CLOCK DATA
;*******************************************************************************
```

```
;                              KW11-K CLOCK B DATA                              *
;                                                                               *
;                                                                              ***
;                                                                               *

        K11CSR  =       170432          ;KW11-K CONTROL STATUS REGISTER
        K11BR   =       170434          ;KW11-K BUFFER REGISTER
        K11IV   =       364             ;KW11-K INTERRUPT VECTOR ADDRESS
        GOBIT   =       1               ;SETTING GOBIT STARTS CLOCK
        INTOV   =       100             ;ENABLE INTERRUPT ON OVERFLOW
        FREQ    =       4               ;SET CLOCK B INTERNAL FREQ TO 100 KHZ
        OVFLAG  =       200             ;FLAG BIT, IT IS SET AFTER OVERFLOW
                                        ;AND MUST BE CLEARED AFTER INTERRUPT

;                                                                               *
;                                                                              ***
;                                                                               *
;                                                                               *
;                                                                               *
;*******************************************************************************
;
;       THE PURPOSE OF THIS SEGMENT IS TO SET UP THE KW11-K REALTIME
;       CLOCK B TO GENERATE PERIODIC INTERRUPTS (PRESET IN DATA BLOCK)
;       DURING WHICH THE INTERRUPT SERVICE ROUTINE IS EXECUTED
;
        .SBTTL  SETUP CLOCK

CLKSET: MOV     #CLKINT,@#K11IV         ;PUT IRS INTO VECTOR ADDRESS
        MOV     #340,@#K11IV+2          ;SET VECTOR PRIORITY TO PR7
        MOV     #RATE,@#K11BR           ;DOWN COUNTER TO ??? FOR 1KHZ
        BIS     #FREQ,@#K11CSR          ;SET FREQ TO 100 KHZ
        BIS     #INTOV,@#K11CSR         ;ENABLE INTERRUPT
        CLR     @#177546                ;STOP LINE CLOCK
        BR      DRSET           ;GO ON TO SET UP DR11

;*******************************************************************************

; THIS SECTION SETS UP THE DR11 FOR GENERATION INTERRUPTS FROM FURNACE
; TRIGGER OR THE FOOT PEDAL.
; THE INTERRUPT IS GENERATED WHEN PIN RR OR NN OF J1 I/O PORT GOES LOW
; THE SERVICE ROUTINE IMMEDIATELY DISABLES THE INTERRUPT AND CONTINUES
; IN THE WAIT LOOP, MAKING THE INTERRUPT A ONE SHOT DEAL
;
;
        DRCSR   =       167770  ;CSR FOR DR11
        DINTV   =       300     ;INTERRUPT VECTOR A
        INTENB  =       100     ;INTERRUPT A ENABLE
        INTGEN  =       200     ;INTERRUPT A GENERATE
        PRIORT  =       4       ;PRIORTY LEVEL FOR DR11
;
;
DRSET:  MOV     #DINTV,R1               ;R1=INTERRUPT VECTOR ADDRESS
        MOV     #DRINT,(R1)             ;LOAD DR11 SERVICE ROUTINE VECTOR
        BIS     #INTENB,@#DRCSR         ;ENABLE INTERRUPT A
;       .PRINT  #READY                  ;PRINT READY MESSAGE AND WAIT
        BR IDLE         ;BRANCH TO MAIN LOOP

READY:  .ASCIZ  'READY FOR DR11 TRIGGER'<12><15>
        .EVEN

;*******************************************************************************
;                                                                               *
;                                                                              ***
;                                                                               *
; DR11 INTERRUPT SERVICE ROUTINE: UPON EXTERNALLY GENERATED INTERRUPT,
```

```
; THIS ROUTINE IS ENTERED STARTING THE KW11-K CLOCK, AND DISABLING THE
; DR11 INTERRUPT UNTIL A NEW CALL FROM MAIN BEGINS THE ENTIRE ACQSUB
; SEQUENCE OVER AGAIN

DRINT:  .TTYOUT #7                      ;BELL INDICATES ISR ENTRY
        MOV     #4000,@#DAC1A           ;OUTPUT VOLTAGE
        BIC     #INTENB,@#DRCSR         ;DISABLE INTERRUPT A
        BIS     #GOBIT,@#K11CSR         ;SET GOBIT TO START CLOCK
        RTI                     ;GO ON TO MAIN PROG LOOP
;                                                                       *
;                                                                      ***
;                                                                       *
;***********************************************************************


        .SBTTL  MAIN LOOP
;       THE PURPOSE OF THIS SEGMENT IS TO WAIT IN A LOOP, CHECKING TO
;       SEE IF THE BUFFER IS FULL, JUMPING TO THE WRITE SUBROUTINE
;       WHEN THE BUFFER DOES FILL UP. MEANWHILE DATA IS BEING TAKEN BY
;       INTERRUPT SERVICE ROUTINE AND GOING INTO THE SECOND BUFFER.
;       THE PROGRAM FLIP-FLOPS BETWEEN THE TWO, WRITING DATA INTO THE
;       'EMPTY' ONE, AND WRITING DATA OUT TO DISK FROM THE 'FULL' ONE.
;       THE FLIPFLOP CONTINUES UNTIL THE BLKCTR INDICATES THE TOTAL
;       DATA SET TO BE ACQUIRED FOR ONE SAMPLE IS WRITTEN TO DISK,
;       AND THEN EXITS ACQSUB FOR RETURN TO MAIN CALLING PROGRAM.
;
IDLE:   CMP     BLKCTR,@#FILSIZ ;TEST FILE FULL
        BHIS    CLOSE           ;CLOSE IF FILE FULL
        TSTB    BFRFUL                  ;TIGHT LOOP WHILE
        BPL     IDLE                    ;TESTING BUFFER FULL?
        JSR     PC,WTLOOP       ;BRANCH TO WRITE IF FULL
        BR      IDLE            ;LOOP IF NOT FULL


;       THIS SECTION OF CODE CLOSES THE I/O CHANNEL

CLOSE:  CLR     @#K11CSR        ;STOP CLOCK
        MOV     #100,@#177546   ;RESTART LINE CLOCK
        .CLOSE  #3      ;CLOSE CHANNEL
;       .PRINT  #DONE   ;PRINT DONE MESSAGE
        MOVB    #-62.,MVINDX    ;RESTORE STARTING VALUE
                                ;NOT NEC. IN STANDALONE BUT FOR
                                ;CALLABLE SUBROUTINE WITHOUT THIS
                                ;REFRACTOR PLATE SHIFT DIFFERS RUN TO RUN
        ;.SRESET                ;SOFTWARE RESET- OK IN STANDDALONE, BUT
                                ;CREATES ERROR IN SECOND PASS OF FORTRAN
                                ;PROGRAM CALLING THIS SUBR. FOR REPEAT RUNS
        RTS     PC              ;EXIT PROGRAM


        .SBTTL  INTERRUPT SERVICE ROUTINE
;
;
;***********************************************************************
;                       AD11-K DATA                                     *
;                                                                       *
;                                                                      ***
;                                                                       *
        ADSR1 = 170400  ;ADC1 STATUS REGISTER
        ADBR1 = 170402  ;ADC1 BUFFER REGISTER
        DAC1A  = 170420 ;DAC A REGISTER ON AD11-K #1
        FLAG  = 200     ;SIGN BIT MASK FOR BYTE FLAGS
        NOCHNS = 16.    ;NUMBER OF CHANNELS
;
;
;                       MODULATION VOLTAGE TABLE
```

```
;
MVINDX: .BYTE   -62.    ;MOD VOLTAGE TABLE INDEX
        .EVEN

MVTABL: .WORD   3237,3547,4000,4000     ;MODULATION VOLTAGE TABLE
        .WORD   4000,4000,4000,4000
        .WORD   6203,7173,7526,7666
        .WORD   7777,5670,5214,4704
        .WORD   4540,4230,4000,4000
        .WORD   4000,4000,4000,4000
        .WORD   1575,0605,0251,0112
        .WORD   0000,2063,2510,3075

;                                                                              *
;                                                                             ***
;                                                                              *
;                                                                              *
;*******************************************************************************

;.PSECT CODE
;       THE PURPOSE OF THIS SEGMENT IS TO INITIATE 16 CONVERSIONS ON THE
;       ANALOG-DIGITAL CONVERTER, PLACING THE DATA INTO THE BUFFER.
;       (ONE CONVERSION PER CHANNEL)
;

CLKINT: MOV     R0,-(SP)        ;SAVE REGISTERS R0,R1,R2,R3
        MOV     R1,-(SP)
        MOV     R2,-(SP)
        MOV     R3,-(SP)
        MOV     #NOCHNS,R2      ;R2=NUMBER OF CHANNELS
        MOV     POINTR,R1       ;R1=NEXT FREE ADDRESS IN BUFFER
        CLR     @#ADSR1         ;CLEAR ADC STATUS REGISTER

        LOOP:   INC     @#ADSR1         ;START CONV ON ADC1

                WAIT1:  TSTB @#ADSR1    ;TEST DONE BIT ADC1
                        BPL WAIT1

                MOV     @#ADBR1,(R1)+           ;MOVE DATE TO BUFFER
                ADD     #400,@#ADSR1            ;INC CHAN ADC1

                SOB     R2,LOOP                 ;LOOP FOR NEXT CHANNEL

                                ;THIS SECTION RETRIEVES THE MODULATION
                                ;TABLE VOLTAGE INDEX, OUTPUTS THE VOLTAGE
                                ;AT THE DAC, STEPS THE INDEX FORWARD,
                                ;UPDATES AND RESETS AS NECESSARY

        MOVB    MVINDX,R3       ;R3=MOD VOLTAGE TABLE INDEX
        MOV     MVTABL+64.(R3),@#DAC1A  ;UPDATE OUTPUT VOLTAGE
        ADD     #2,R3           ;STEP INDEX FORWARD
        BLT     NOREST          ;BRANCH IF INDEX RESET NOT NECESSARY
        MOV     #-64.,R3        ;RESET MOD VOLT INDEX
NOREST: MOVB    R3,MVINDX       ;SAVE UPDATED INDEX

        MOV     R1,POINTR       ;UPDATE POINTER
        CMP     CUREND,R1       ;TEST END OF BUFFER
        BHI     INTREX          ;BR IF NOT FULL TO EXIT INTERRUPT

        MOVB    #-1,BFRFUL      ;SET BUFFER FULL FLAG
        TSTB    BUFIND          ;WHICH BUFFER  FULL?
        BGT     CLK020          ;BR IF BUFFER 1

        INCB    BUFIND          ;SET BUFFER INDICATER TO BUFF1
        MOV     BF1ADR,POINTR   ;BUFFER POINTER = BUFFER 1 ADDRESS
        MOV     BF1END,CUREND   ;CURRENT END = BUFFER 1 END
```

```
        MOV     BF0ADR,WRTBFR   ;WRITE BUFFER = BUFFER 0 ADDRESS
        BR      INTREX          ;EXIT INTERRUPT

CLK020: DECB    BUFIND          ;SET BUFFER INDICATOR TO BUFF0
        MOV     BF0ADR,POINTR   ;BUFFER POINTER = BUFFER 0 ADDRESS
        MOV     BF0END,CUREND   ;CURRENT END = BUFFER 0 END
        MOV     BF1ADR,WRTBFR   ;WRITE BUFFER = BUFFER 1

        INTREX: MOV     (SP)+,R3        ;RESTORE REGISTERS
                MOV     (SP)+,R2
                MOV     (SP)+,R1
                MOV     (SP)+,R0


        BIC     #OVFLAG,@#K11CSR        ;CLEAR OVERFLOW FLAG
        BIS     #GOBIT,@#K11CSR         ;RESETS GO BIT

        RTI                             ;RETURN TO INTERRUPTED PROG


;       THIS SECTION OF CODE INITIATES WRITE

WTLOOP: CLRB    BFRFUL                                  ;CLEAR BUFFER FULL INDICATOR
        .WRITE  #EM1,#3,WRTBFR,#WRDCNT,BLKCTR           ;WRITE DATA FROM BUFFER
        BCS     FAILW                                   ;BR IF WRITE FAILED
        ADD     #BUFSIZ,BLKCTR                          ;UPDATE BLOCK COUNTER
        RTS     PC              ;RETURN TO DATA ACQUISITION SEGMENT


FAILW:  .PRINT #FW              ;PRINT / WRITE FAILED /
        RTS     PC



.END
```

```
.TITLE AVERAGE THE INTENSITIES IN FILE1.DAT; SAVE GRPAVG AND GRNDAV
.IDENT  /AVGSUB/
.GLOBL  AVGSUB
.MCALL  .LOOKUP,.ENTER,.READW,.WRITW,.CLOSE
.MCALL  .PRINT,.EXIT
;
;EDIT OF WTAVG TO REMOVE OVERFLOW ERROR IN THE FORMER
;WITH OVERFLOW AVG ALMOST BUT NOT EXACTLY CORRECT
;AND GRPAVG IS INACCESSIBLE SINCE OVERFLOW SETS SIGN BIT MAKING RESULT NEG.
;AND FURTHER EDIT TO CALLABLE SUBROUTINE FOR CALL FROM FLAME
;
ERRBYT=52
AVGSUB:
START:  .LOOKUP #AREA,#10.,#FL1SPC      ;LOOKUP DATA FILE
        BCS     5$                      ;BRANCH IF NOT FOUND
        MOV     R0,R3                   ;COPY FILE SIZE TO R3
        .ENTER  #AREA,#8.,#FL2SPC,R3    ;CREATE TEMP FILE SAME SIZE
        BCS     6$                      ;BRANCH IF ENTER FAILS
        .ENTER  #AREA,#9.,#FL3SPC,R3
        BCS     7$
        CLR     BLK                     ;INITIALIZE BLOCK NO TO 0
        MOV     ENDBUF,R4               ;AND CLEAR GRNDAV BUFFER
        MOV     #AVGBUF,R2
3$:     CLR     (R2)+
        SOB     R4,3$
        MOV     ENDBUF,R4
        MOV     #INTBUF,R2              ;ALSO CLEAR INTBUF
4$:     CLR     (R2)+
        SOB     R4,4$
        JMP     GO                      ;START AVERAGING CYCLE
5$:     MOV     #NOFIL,R0               ;IF LOOKUP ERROR PRINT
        JMP     PR                      ;MESSAGE AND EXIT
6$:     MOV     #NOENT,R0               ;DITTO OPEN ERROR
        JMP     PR
7$:     MOV     #NOENT1,R0
        JMP     PR
;
;AVERAGING CYCLE BEGINS HERE
;DATA IS READ FOR ONE PASS OVER MODULATION INTERVAL AND SUMMED INTO INTBUF
;32 PASSES CONSTITUTE ONE GROUP; 8 GROUPS LEAD TO GRNDAV
;
GO:     MOV     #32.,R5
GO1:    MOV     #BUFFER,R1
        .READW  #AREA,#10.,#BUFFER,#512.,BLK     ;READ A BLOCK
        BCC     3$                      ;BRANCH IF READ SUCCEEDS
        TSTB    @#ERRBYT                ;WAS FAIL ERROR AN END-OF-FILE?
        BNE     2$                      ;IF NO BRANCH TO ERROR OUT
        JMP     CLOS                    ;  ELSE BRANCH TO CLOSE
2$:     MOV     #RERR,R0                ;MOVE HARD READ ERROR MSG TO R0
        BR      PR                      ;  AND PRINT MSG OUT
3$:     MOV     ENDBUF,R4
        MOV     #INTBUF,R2
4$:     ASR     (R1)                    ;DIVIDE DATA BY 4 BEFORE SUMMING
        ASR     (R1)                    ;FOR GRP SUM TO AVOID OVERFLOW
        ADD     (R1)+,(R2)+             ;SUM FOR GRP SUM
        SOB     R4,4$                   ; AND REPEAT FOR ALL DATA IN SET
        ADD     #2,BLK                  ;INCREMENT BLK CTR FOR NEXT OF 32 SETS
        SOB     R5,GO1                  ;AND LOOP UNTIL ALL 32 PROCESSED
        MOV     #INTBUF,R2
        MOV     ENDBUF,R4
        MOV     #AVGBUF,R3
AVG:    ASR     (R2)
        ASR     (R2)
        ASR     (R2)                    ;CALC GRP MEAN AND ADD TO GRND SUM
        ADD     (R2)+,(R3)+
```

```
        SUB     R4,AVG
        .WRITW  #AREA,#8.,#INTBUF,#512.,BLK1    ;WRITE AVGS JUST CALC
        ADD     #2,BLK1                         ;AND INCREMENT BLOCK COUNTER
        BLC     NXTPAS                          ;BRANCH IF WRITE SUCCEEDS
        MOV     #WERR,R0                        ; ELSE MOVE HARD WRITE ERROR MSG TO R0
        BR      PR                              ; AND PRINT ERROR MESSAGE
NXTPAS: MOV     ENDBUF,R4                       ;CLEAR REUSABLE INTBUF BEFORE NEXT GR
        MOV     #INTBUF,R2
CLR2:   CLR     (R2)+
        SOB     R4,CLR2
        JMP     GO                              ;AND JUMP TO START OF GROUP AVG LOOP
CLOS:   .CLOSE  #10.
        .CLOSE  #8.                             ;CLOSE TEMP FILE; MAKE PERMANENT
        CLR     BLK1                            ;RESET CTR- REUSE NOT APPEND FILE
;       MOV     #DONE,R0                        ;DONE MSG TO R0
;       .PRINT                                  ; AND PRINT MESSAGE OUT
        MOV     ENDBUF,R4
        MOV     #AVGBUF,R3
;
;ALL GROUP MEANS HAVE BEEN CALCULATED AND SUMMED INTO GRNDAV BUFFER
;THIS PROGRAM SEGMENT CALCULATES THE GRAND MEANS OF 512 INTENSITIES
;32 REFRACTOR PLATE POSITIONS FOR EACH OF 16 CHANNELS
;
GRNDAV: ASR     (R3)
        ASR     (R3)
        ASR     (R3)+
        SOB     R4,GRNDAV
        .WRITW  #AREA,#9.,#AVGBUF,#512.,BLK2
        BCC     CLOS2
        MOV     #WERR1,R0
        BR      PR
CLOS2:  .CLOSE  #9.
;       MOV     #DONE1,R0
        BR      FINISH
PR:     .PRINT
FINISH: RTS     PC
AREA:   .BLKW   5
BLK:    .WORD   0
BLK1:   .WORD   0
BLK2:   .WORD   0
BUFFER: .BLKW   512.                            ;I/O BUFFER = 1 BLOCK
INTBUF: .BLKW   512.
AVGBUF: .BLKW   512.
ENDBUF: .WORD   512.
FL1SPC: .RAD50 /DL1/                            ;READ FILE SPEC
        .RAD50  /FILE1/
        .RAD50  /DAT/
FL2SPC: .RAD50  /DL1/                           ;WRITE FILE SPEC
        .RAD50  /GRPAVG/
        .RAD50  /DAT/
FL3SPC: .RAD50  /DL1/
        .RAD50  /GRNDAV/
        .RAD50  /DAT/
NOFIL:  .ASCIZ  /FILE1.DAT NOT FOUND/
NOENT:  .ASCIZ  /ENTER FAILED-GRPAVG.DAT/
NOENT1: .ASCIZ  /ENTER FAILED-GRNDAV.DAT/
WERR:   .ASCIZ  /WRITE ERROR GRPAVG/
WERR1:  .ASCIZ  /WRITE ERROR GRNDAV/
RERR:   .ASCIZ  /FILE1 READ ERROR/
DONE:   .ASCIZ  /GROUP AVERAGES DONE COMPLETED/
DONE1:  .ASCIZ  /GRAND AVERAGES DONE/
        .EVEN
        .END START
```

```
      SUBROUTINE CALSUB
C
C     SUBROUTINE WILL CALCULATE  FIVE ABSORBANCES.
C
C     DATA WILL FIRST BE ACQUIRED USING THE MACRO ALOGAU AND WILL NEXT BE
C     AVERAGED USING THE MACRO WRTAV. RDFILE.FOR WILL READ THE
C     AVERAGED DATA FILE, ORDER IT, AND THEN CALL THIS SUBROUTINE
C
      DIMENSION EL(16),ABS(6)
      INTEGER DATA(32)
      COMMON /BUFS/ DATA,ABS
C
C     THE USE OF COMMON FOR VARIABLES USED BOTH BY SUBROUTINE AND MAIN
C     ELIMINATES ANY NEED TO PASS THESE VARIABLES

      DATA EL(1),EL(2),EL(3),EL(4)/2HIE,2HZN,2HCD,2HSB/
      DATA EL(5),EL(6),EL(7),EL(8)/2HBI,2HBE,2HCO,2HMO/
      DATA EL(9),EL(10),EL(11),EL(12)/2HCR,2HCU,2HSN,2H V/
      DATA EL(13),EL(14),EL(15),EL(16)/2HMN,2HAG,2HFE,2HNI/
      REAL LN0,LN1,LN2,LN3,LN4,LN5,LN6,LNSENS,LNSTR
C
C     CLEAR ABSORBANCE ARRAY
C
      DO 15 I=1,6
            ABS(I)=0.00
15    CONTINUE
C
C     CALCULATE BG AND LINE INTENSITIES FOR ABSORBANCES-- MOST SENSITIVE
C
      BG0=DATA(1)+DATA(2)+DATA(3)+DATA(4)
      BG1=DATA(13)+DATA(14)+DATA(15)+DATA(16)
      BG2=DATA(17)+DATA(18)+DATA(19)+DATA(20)
      BG3=DATA(29)+DATA(30)+DATA(31)+DATA(32)
      BGSENS=BG0+BG1+BG2+BG3
      LN0=DATA(5)+DATA(6)+DATA(7)+DATA(8)
      LN1=DATA(9)+DATA(10)+DATA(11)+DATA(12)
      LN2=DATA(21)+DATA(22)+DATA(23)+DATA(24)
      LN3=DATA(25)+DATA(26)+DATA(27)+DATA(28)
      LNSENS=LN0+LN1+LN2+LN3
C
C     AND OTHERS
C
      BG=DATA(1)+DATA(16)+DATA(17)+DATA(32)+1
      BG1=DATA(16)+DATA(32)+1
      LN2=DATA(5)+DATA(12)+DATA(21)+DATA(28)+1
      LN3=DATA(4)+DATA(13)+DATA(20)+DATA(29)+1
      LN4=DATA(3)+DATA(14)+DATA(19)+DATA(30)+1
      LN5=DATA(2)+DATA(15)+DATA(18)+DATA(31)+1
      LN6=DATA(1)+DATA(17)
C
C     STRAY LIGHT CORRECTION TESTS
C
      BGSTR=DATA(1)+DATA(16)+DATA(17)+DATA(32)
      LNSTR=DATA(8)+DATA(9)+DATA(24)+DATA(25)+1
      TEST=ALOG10(BGSTR/LNSTR)
C
C     ABSORBANCE CALCULATIONS
C
      ABS(1)=ALOG10(BGSENS/LNSENS)
      ABS(2)=ALOG10(BG/LN2)
      ABS(3)=ALOG10(BG/LN3)
      IF (TEST .GE. 0.7)GO TO 20
      ABS(4)=ALOG10(BG/LN4)
      ABS(5)=ALOG10((BG/2.)/LN5)
      ABS(6)=ALOG10((BG1)/LN6)
```

```
      GO TO 30
C
C     ABSORBANCES NEEDING STRAY LIGHT CORRECTION
C
20    CORR=DATA(9)+DATA(24)
      BG=BG-(2.*CORR)
      BG1=BG1-CORR
      LN4=LN4-(2.*CORR)
      LN5=LN5-2.*CORR
      LN6=LN6-CORR
      IF(BG .LE. 0.0)GO TO 27
      IF(LN4 .LE. 0.0)GO TO 25
      ABS(4)=ALOG10(BG/LN4)
25    IF(LN5 .LE. 0.0)GO TO 27
      ABS(5)=ALOG10(BG1/LN5)
27    IF(BG1 .LE. 0.0)GO TO 30
      IF(LN6 .LE. 0.0)GO TO 30
      ABS(6)=ALOG10(BG1/LN6)
C
C     PRINT OUT RESULTS AFTER RETURN TO MAIN
C
30    CONTINUE
      RETURN
      END
```

```
      PROGRAM FLMDAT
C
C       THIS PROGRAM FIRST CALLS ACQSUB.MAC TO COLLECT THE DATA WHICH
C       CONSTITUTES DL1:FILE1DAT
C       THEN CALLS AVGSUB.FOR WHICH READS THAT FILE AND AVERAGES IT
C        TO GIVE EIGHT GROUP AVERAGES OF 32 IN GRPAVG.DAT AND
C        GRAND MEAN ALL CHANNELS,ALL POSITIONS IN GRNDAV.DAT
C       NEXT REORDERS GROUP AVG DATA FOR ABSORBANCE CALCULATIONS
C       CALLING CALSUB.FOR TO PERFORM THE CALCULATIONS
C       FINALLY  AVERAGES GROUP ABS. AND CALCULATES SIGMA(ABS) FOR S/N RATIO
C       THEN LOGS THE CALC GRAND MEAN ABSORBANCES AND SIGMAS IN DL1:ABSORB.DAT
C        WITH GROUP ABSORBANCES IN DL1:GRPABS.DAT
C       THEN LOOPS TO BEGINNING FOR NEXT SAMPLE TO A MAXIMUM DEFINED BY MAXRUN
C
C       BECAUSE OF THE NUMBER OF FILES WHICH THIS PROGRAM REQUIRES OPEN AT
C       ONCE, IT MUST BE COMPILED WITH THE /UNITS:10 SWITCH
C       IE  FORTRAN/UNITS:10 FLMDAT
C       THEN  LINK FLMDAT,ACQSUB,AVGSUB,CALSUB,SYSLIB,FORLIB
C
        DIMENSION IDATA(512),IBUF(16,32),IND(16)
        DIMENSION SUMABS(6),SQSUM(6)
        REAL ABSORB(16,6),ABS(6),SIGMA(16,6)
        EQUIVALENCE (IDATA(1), IBUF(1))
        COMMON  /BUFS/ IBUF,ABS
        COMMON /BUFR/ IND
        INTEGER IBUF(32),WCNT
        BYTE EL(32)
        DATA EL(1),EL(2),EL(3),EL(4)/1HT,1HE,1HC,1HN/
        DATA EL(5),EL(6),EL(7),EL(8)/1HC,1HD,1HS,1HR/
        DATA EL(9),EL(10),EL(11),EL(12)/1HB,1HI,1HR,1HC/
        DATA EL(13),EL(14),EL(15),EL(16)/1HC,1HD,1HM,1HU/
        DATA EL(17),EL(18),EL(19),EL(20)/1HC,1HR,1HS,1HN/
        DATA EL(21),EL(22),EL(23),EL(24)/1HC,1HU,1H ,1HV/
        DATA EL(25),EL(26),EL(27),EL(28)/1HM,1HN,1HA,1HG/
        DATA EL(29),EL(30),EL(31),EL(32)/1HP,1HB,1HN,1HI/
C
C       SET UP ACTIVE CHANNELS AND INDICATE CHANNEL FORK MONITORING
C
        DO 1, I=1,16
                IND(I)=1
                TYPE *,' IS CHANNEL ',I,' ACTIVE?'
                ACCEPT 1503,YESNO
                IF (YESNO .EQ. 'N')IND(I)=0
1       CONTINUE
        IF (IND(11) .EQ. 1) IMON=11
2       TYPE *,'MONITOR CHANNEL OTHER THAN CU??'
        ACCEPT 1503,YESNO
        IF (YESNO .NE. 'Y' .AND. YESNO .NE. 'N')GO TO 2
        IF (YESNO .EQ. 'Y') TYPE *,'ENTER NO. FOR MONITOR CHANNEL'
        IF (YESNO .EQ. 'Y')ACCEPT 1503,IMON
3       TYPE *, 'ENTER MAXIMUM NO. SAMPLES FOR DATA COLLECTION RUN'
        ACCEPT *,MAXRUN
C
C       OPEN REQUIRED OUTPUT FILES
C
        OPEN (UNIT=11,TYPE='NEW',ACCESS='DIRECT',NAME='DL1:ABSORB.DAT',
     1    RECORDSIZE=16)
        OPEN (UNIT=12,TYPE='NEW',ACCESS='DIRECT',NAME='DL1:GRPABS.DAT',
     1     RECORDSIZE=8)
C
C       DL1:SIMAAC.DAT RECORD IS 6 ABSORBANCES AND 6 SIGMAS AS REAL DATA
C        SO RECSIZ=16
C       DL1:GRPABS.DAT RECORD IS 6 ABSORBANCES AS REAL NUMBERS SO RECSIZ=8
C
C       PRINT EXPERIMENT HEADERS,INITIALIZE I/O COUNTERS
```

```
C
5       PRINT 1500
        PRINT 1501
        ICNT=1
        NCNT=1
        WCNT=1
        IBLK=1
        DO 1000 KK=1,MAXRUN
C
C       FOR EACH RUN CALL SUBROUTINES TO COLLECT,AVERAGE AND STORE THE
C       RAW INTENSITY DATA
C
                TYPE *, 'READY FORR TRIGGER'
                CALL ACQSUB
                CALL AVGSUB
C
C       READ STORED DATA BACK IN IN ORDER TO
C       CALCULATE ABSORBANCE FOR EACH SET OF BOXCAR AVERAGED INTENSITIES
C       ONE CHANNEL IS PROCESSED AT A TIME
C       BECAUSE FORMATTING FOR ALL CHANNELS EXCEEDS ALLOWABLE MEMORY
C
           PRINT 1502,KK
           OPEN (UNIT=3,TYPE='OLD',ACCESS='DIRECT',NAME='DL1:GRPAVG.DAT',
     1      RECORDSIZE=256)
C       GRPAVG STORED AS INTEGERS (512)= 256 DOUBLE WORDS GIVES RECSIZ
           DO 200 ICH=1,16
              IF (IND(ICH) .EQ. 0) GO TO 200
              DO 10 N=1,6
                SUMABS(N)=0.0
                SQSUM(N)=0.0
10            CONTINUE
              DO 80 NUGRP=1,8
                READ (3 'IBLK)(IDATA(I),I=1,512)
                DO 35,IPOS=1,14
                        JJ=IPOS+18
                        IBUF(JJ)=IBUF(ICH,IPOS)
35              CONTINUE
                DO 36,IPOS=15,32
                        JJ=IPOS-14
                        IBUF(JJ)=IBUF(ICH,IPOS)
36              CONTINUE
                CALL CALSUB
                WRITE (12 'WCNT) (ABS(N),N=1,6)
                IBLK=IBLK+1
                WCNT=WCNT+1
                DO 50 N=1,6
                        SUMABS(N)=SUMABS(N)+ABS(N)
                        SQSUM(N)=SQSUM(N)+ABS(N)**2
50              CONTINUE
80            CONTINUE
              DO 90 N=1,6
                ABSORB(ICH,N)=SUMABS(N)/8.
                SIGMA(ICH,N)=SQRT (SQSUM(N)-(SUMABS(N)**2)/8.)/7.
90            CONTINUE
                IF (ICH .EQ. IMON)TYPE 3005,KK,(ABSORB(ICH,N),N=1,6)
                WRITE (11 'NCNT)((ABSORB(ICH,N),SIGMA(ICH,N)),N=1,6)
                NCNT=NCNT+1
                K=ICH*2
                IBLK=1
                PRINT 3000,((EL(J),J=K-1,K),(ABSORB(ICH,N),
     1            SIGMA(ICH,N),N=1,6))
200        CONTINUE
           CLOSE (UNIT=3)
C
C       NEXT PROGRAM SEGMENT SAVES FINAL AVERAGED INTENSITIES FOR ALL SAMPLE
C       RUNS OF AN EXPER FOR USE WITH ABSORBANCE/INTENSITY PLOTTING PROGRAMS
```

```
C       AND FOR THE CALCULATION OF ABSORBANCES USING THE ALTERNATE ALGORITHM
C       IN ALTCAL
C
           OPEN (UNIT=4,TYPE='OLD',ACCESS='DIRECT',NAME='DL1:GRNDAV.DAT',
     1       RECORDSIZE=256)
           OPEN (UNIT=13,TYPE='NEW',ACCESS='DIRECT',NAME='DL1:INTENS.DAT',
     1       RECORDSIZE=16)
           READ (4 '1)(IDATA(I),I=1,512)
           DO 300 ICH=1,16
                IF (IND(ICH) .EQ. 0)GO TO 300
                DO 250 IPOS=1,14
                        JJ=IPOS+18
                        TBUF(JJ)=IBUF(ICH,IPOS)
250             CONTINUE
                DO 260 IPOS=15,32
                        JJ=IPOS-14
                        TBUF(JJ)=IBUF(ICH,IPOS)
260             CONTINUE
                WRITE (13 'ICNT)(TBUF(JJ),JJ=1,32)
                ICNT=ICNT+1
300        CONTINUE
           CLOSE (UNIT=4)
           CLOSE (UNIT=13)
1000    CONTINUE
        CLOSE (UNIT=11)
        CLOSE (UNIT=12)
        STOP
C
1500    FORMAT (/T39,'SIMAAC ANALYSES: CALCULATED ABSORBANCES')
1501    FORMAT (//7X,'EL',/X,'ABS1',4X,'SIGMA1',4X,'ABS2',4X,
     1    'SIGMA2',4X,'ABS3',4X,'SIGMA3',4X,'ABS4',4X,
     1    'SIGMA4',4X,'ABS5',4X,'SIGMA5',4X,'ABS6',4X,'SIGMA6')
1502    FORMAT (/3X,'RUN ',12)
1503    FORMAT(A1)
3000    FORMAT (7X,2A1,5X,12(F7.4,2X))
3005    FORMAT (2X,I2,3X,6(F7.4,2X))
        END
```

SEE APPENDIX 3 FOR ALL CALLED SUBROUTINES

APPENDIX 4

```
      PROGRAM FUNN
C
C       THIS PROGRAM FIRST CALLS ACQSUB TO COLLECT THE DATA WHICH
C       CONSTITUTES DU1:FILE1.DAT
C       NEXT REQUIRES DATA FOR ABSORBANCE CALCULATIONS
C       CALLS CALHGA TO PERFORM THE ABSORBANCE CALCULATIONS FOR
C       EACH PASS ACROSS THE MODULATION INTERVAL IN SEQUENCE,
C       THEN COMPARES LATEST ABSORB WITH PEAK TO ESTABLISH
C       PEAK HT ABSORB AND ALSO SUMS LATEST WITH ALL PREV
C       FOR PEAK AREA ABSORB -- THREE CALIBRATION CURVES
C       FINALLY LOCS PEAK LOCATION AND THE THREE CALCULATED
C       HT AND AREA ABSORBANCES IN HGAABS.DAT
C       AND LOOPS FOR NEXT SAMPLE TO A MAXIMUM DEFINED BY MAXRUN
C       (CANNOT EXCEED 99 AS PER FORMAT FOR FUN NO. PRINT STATEMENT)
C
      DIMENSION IDATA(512),IBUF(16,32),IND(16)
      DIMENSION AREA(16,6),ABS(6),IMAX(16)
      REAL HT(16,6)
      EQUIVALENCE (IDATA(1),IBUF(1,1))
      COMMON /BUFS/ IBUF,ABS
      INTEGER KCNT,IBUF(32)
      BYTE EL(40)
      DATA EL(1),EL(2),EL(3),EL(4)/1HI,1HF,1HV,1HN/
      DATA EL(5),EL(6),EL(7),EL(8)/1HC,1HD,1HS,1HK/
      DATA EL(9),EL(10),EL(11),EL(12)/1HB,1HI,1HR,1HP/
      DATA EL(13),EL(14),EL(15),EL(16)/1HC,1HO,1HM,1HU/
      DATA EL(17),EL(18),EL(19),EL(20)/1HC,1HK,1HS,1HN/
      DATA EL(21),EL(22),EL(23),EL(24)/1HC,1HU,1H ,1HV/
      DATA EL(25),EL(26),EL(27),EL(28)/1HM,1HN,1HA,1HG/
      DATA EL(29),EL(30),EL(31),EL(32)/1HF,1HB,1HN,1HI/
      DATA EL(33),EL(34),EL(35),EL(36)/1HF,1HO,1HM,1HI/
      DATA EL(37),EL(38),EL(39),EL(40)/1HA,1HU,1HR,1HH/
C
C       SET UP ACTIVE CHANNELS
C
      TYPE *,'PT METALS ANALYZED - YES OR NO?'
      ACCEPT 1499,PTIND
      DO 2 I=1,16
         IND(I)=1
1        TYPE *,'IS CHANNEL ',I,' ACTIVE?'
         ACCEPT 1499,YESNO
         IF (YESNO .EQ. 'N')IND(I)=0
         IF (YESNO .NE. 'Y' .AND. YESNO .NE. 'N')GO TO 1
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 1)EL(1)=EL(33)
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 2)EL(2)=EL(34)
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 3)EL(3)=EL(35)
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 4)EL(4)=EL(36)
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 9)EL(17)=EL(37)
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 9)EL(18)=EL(38)
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 15)EL(29)=EL(39)
         IF(PTIND .EQ. 'Y' .AND. I .EQ. 15)EL(30)=EL(40)
2     CONTINUE
3     IF(IND(11) .EQ. 1)IMON=11
      TYPE *,'MONITOR CHANNEL OTHER THAN CU?'
      ACCEPT 1499,YESNO
      IF (YESNO .NE. 'Y' .AND. YESNO .NE. 'N')GO TO 3
      IF (YESNO .EQ. 'Y')TYPE *,'ENTER MONITOR CHANNEL NO.'
      IF (YESNO .EQ. 'Y')ACCEPT 1504, IMON
C
C
      TYPE *,' ENTER MAXIMUM NO. SAMPLES FOR DATA COLLECTION RUN'
      ACCEPT *,MAXRUN
C
      OPEN (UNIT=11,TYPE='NEW',ACCESS='DIRECT',NAME='DU1:HGAABS.DAT',
```

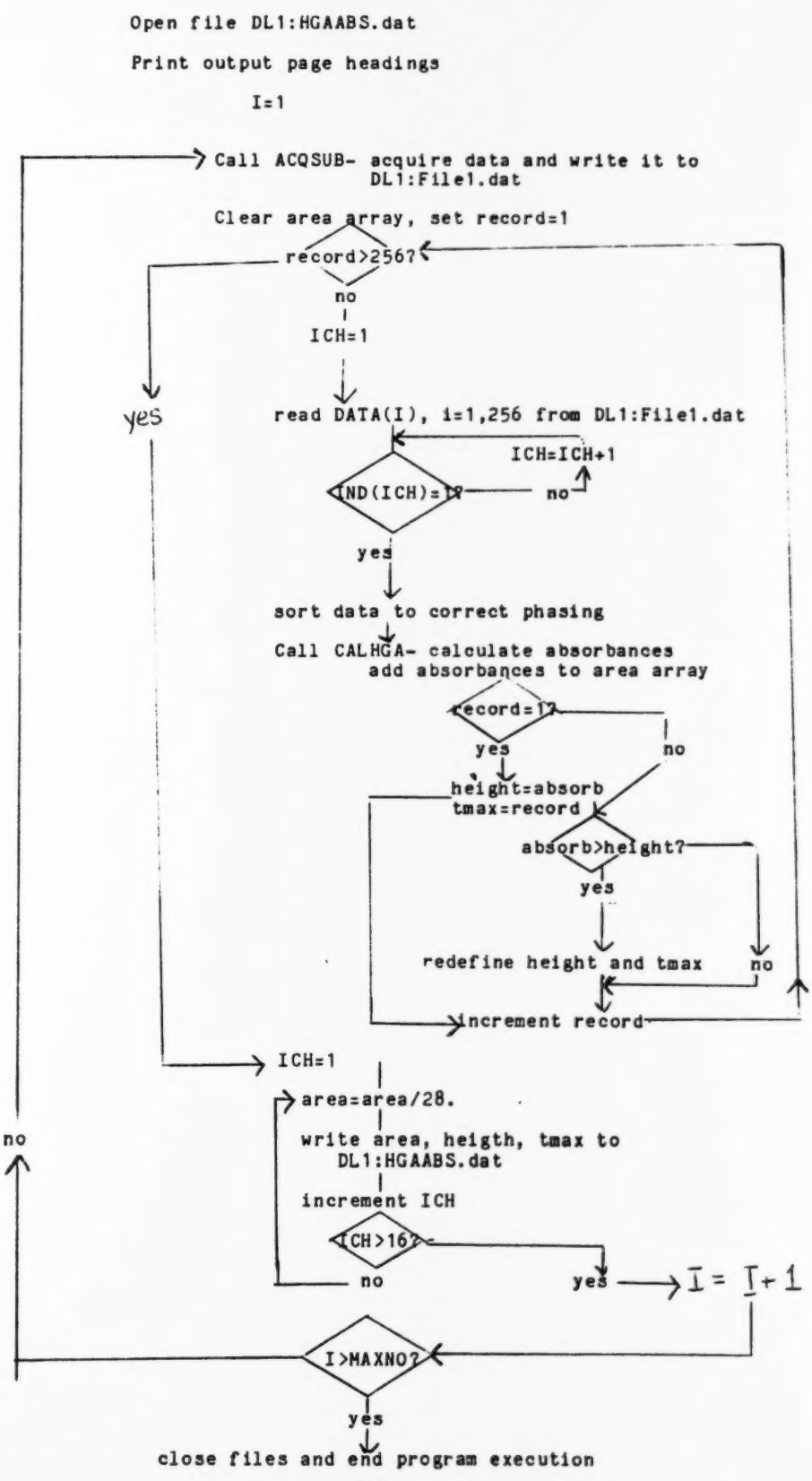
C LINK WITH ACQSUB CALL
C SYSLIB F

```
     1    RECORDSIZE=8)
C       DL1:HGAABS.DAT RECORD IS 1 IMAX, 3  HT ABSORBANCES AS REAL DATA
C        AND 3 AREA ABSORBANCES  SO RECSIZ=8 (7 OF 8 WORDS FILLED)
C
        PRINT 1500
        PRINT 1501
C
        RCNT=1
        NCNT=1
        DO 1000 KK=1,MAXRUN
                TYPE *,'READY FOR TRIGGER'
                CALL ACQSUB
C
C       VOLTAGE INDEX=1 AT A MIDPOINT IN THE MODULATION INTERVAL
C       RESULTING IN DATA ORDER IN DL1:GRNDAV.DAT WHICH IS AWKWARD
C       FOR USE IN ABSORBANCE CALCULATION SUBROUTINE
C       DO 5 AND DO 6 REORDER THE DATA SO THAT IBUF(1) TO IBUF(16)
C       REPRESENT INTENSITY DATA FOR PASS FROM LOWEST TO HIGHEST WAVELENGTH
C       IN THE MODULATION INTERVAL AND IBUF(17) TO IBUF(32) REPRESENT
C       DATA FOR REVERSE DIRECTION PASS
C
                OPEN (UNIT=12,TYPE='OLD',ACCESS='DIRECT',NAME='DL1:FILE1.DAT',
     1           RECORDSIZE=256)
                PRINT 1502,KK
                DO 5,ICH=1,16
                        DO 4 K=1,3
                                AREA(ICH,K)=0.0
4                       CONTINUE
5               CONTINUE
6               READ (12 'RCNT)(IDATA(I),I=1,512)
                        DO 20,ICH=1,16
                                IF (IND(ICH) .EQ. 0) GO TO 20
                                DO 7,IPOS=1,14
                                        JJ=IPOS+18
                                        IBUF(JJ)=IBUF(ICH,IPOS)
7                               CONTINUE
                                DO 8,IPOS=15,32
                                        JJ=IPOS-14
                                        IBUF(JJ)=IBUF(ICH,IPOS)
8                               CONTINUE
                                CALL CALHGA
                                IF (RCNT .NE. 1) GO TO 10
                                DO 9 K=1,3
                                        HT(ICH,K)=ABS(K)
                                        IMAX(ICH)=RCNT
                                        AREA(ICH,K)=AREA(ICH,K)+ABS(K)
9                               CONTINUE
                                IF (RCNT .EQ. 1)GO TO 20
10                              TEST=HT(ICH,1)-ABS(1)
                                IF (TEST .LE. 0)IMAX(ICH)=RCNT
                                DO 11 K=1,3
                                        IF (TEST .LE. 0) HT(ICH,K)=ABS(K)
                                        AREA(ICH,K)=AREA(ICH,K)+ABS(K)
11                              CONTINUE
20                      CONTINUE
                RCNT=RCNT+1
                IF (RCNT .LE. 256)GO TO 6
              DO 30 ICH=1,16
                IF (IND(ICH) .NE. 1) GO TO 30
                JJ=ICH*2
                DO 22 K=1,3
                        AREA(ICH,K)=AREA(ICH,K)/28.
22              CONTINUE
                WRITE (11 'NCNT)IMAX(ICH),(HT(ICH,K),AREA(ICH,K),K=1,3)
                NCNT=NCNT+1
                IF (ICH .EQ. IMON)TYPE 2056, KK,EL(JJ-1),EL(JJ),
```

```
     1            (HT(ICH,K),AREA(ICH,K),K=1,3)
                  PRINT 2050,EL(JJ-1),EL(JJ),TMAX(ICH)
                  PRINT 2055, ((HT(ICH,K),AREA(ICH,K)),K=1,3)
30              CONTINUE
                CLOSE (UNIT=12)
                RCNT=1                                  !RESET TO 1 FOR NEXT RUN
1000        CONTINUE
            CLOSE (UNIT=11)
C
1499        FORMAT (A1)
1500        FORMAT (/130,'FURNACE SIMAAC ANALYSES: HT/AREA ABSORBANCES')
1501        FORMAT (//6X,'EL ',2X,'LOCA. PR',2X,'HT(1)',2X,'AREA1',2X,
         1    'HT(2)',2X,'AREA2',2X,'HT(3)',2X,'AREA3',2X,'HT(4)',2X,
         1    'AREA4',2X,'HT(5)',2X,'AREA5',2X,'HT(6)',2X,'AREA6')
1502        FORMAT (/3X,'RUN ',I2)
1503        FORMAT (6X,2A1,5X,6(F7.4,5X))
1504        FORMAT (I2)
2050        FORMAT (6X,2A1,F5.0)
2055        FORMAT (19X,12F7.4)
2056        FORMAT (5X,I2,2X,2A1,2X,12(F7.4,2X))
            STOP
            END
```

SEE APPENDIX J FOR ACQSUB CALLED BY FURN

ABBREVIATED FLOW DIAGRAM: PROGRAM FURN



```
      SUBROUTINE CALHGA
C
C     SUBROUTINE WILL CALCULATE  THREE ABSORBANCES.
C     SINCE THEY WILL BE THE MOST SENSITIVE THREE, STRAY LIGHT
C     CORRECTIONS ARE NOT NEEDED. LESS SENSITIVE CURVES CANNOT
C     BE USED PROFITABLY DUE TO HIGH CONCENTRATION CARRYOVER
C
C     DATA WILL FIRST BE ACQUIRED USING THE MACRO ACQGAU
C     THE CALLING PROGRAM WILL THEN SORT THE DATA PASS BY
C     PASS ACCROSS THE MODULATION INTERVAL, CALL THIS SUBROUTINE
C     TO COMPUTE ABSORBANCES FROM THE INTENSITIES, RETURN TO
C     MAIN TO SUM ABSORBANCES FOR AREA AND COMPARE TO PREVIOUS
C     PASSES FOR PEAK HEIGHT, AND REPEAT FOR SUCCESSIVE PASSES
C
      DIMENSION EL(16),ABS(6)
      INTEGER DATA(32)
      COMMON /BUFS/ DATA,ABS
C
C     THE USE OF COMMON FOR VARIABLES NEEDED BY BOTH SUBROUTINE AND MAIN
C     ELIMINATES ANY NEED TO PASS THESE VARIABLES
C
      REAL LN0,LN1,LN2,LN3,LN4,LN5,LN6,LNSENS,LNSTR
C
C     CLEAR ABSORBANCE ARRAY
C
      DO 15 I=1,3
            ABS(I)=0.00
15    CONTINUE
C
C     CALCULATE BG AND LINE INTENSITIES FOR ABSORBANCES-- MOST SENSITIVE
C
      BG0=DATA(1)+DATA(2)+DATA(3)+DATA(4)
      BG1=DATA(13)+DATA(14)+DATA(15)+DATA(16)
      BG2=DATA(17)+DATA(18)+DATA(19)+DATA(20)
      BG3=DATA(29)+DATA(30)+DATA(31)+DATA(32)
      BGSENS=BG0+BG1+BG2+BG3
      LN0=DATA(5)+DATA(6)+DATA(7)+DATA(8)
      LN1=DATA(9)+DATA(10)+DATA(11)+DATA(12)
      LN2=DATA(21)+DATA(22)+DATA(23)+DATA(24)
      LN3=DATA(25)+DATA(26)+DATA(27)+DATA(28)
      LNSENS=LN0+LN1+LN2+LN3
C
C     AND OTHERS
C
      BG=DATA(1)+DATA(16)+DATA(17)+DATA(32)+1
      LN2=DATA(5)+DATA(12)+DATA(21)+DATA(28)+1
      LN3=DATA(4)+DATA(13)+DATA(20)+DATA(29)+1
C
C     ABSORBANCE CALCULATIONS
C
      ABS(1)=ALOG10(BGSENS/LNSENS)
      ABS(2)=ALOG10(BG/LN2)
      ABS(3)=ALOG10(BG/LN3)
C
C     PRINT OUT RESULTS AFTER RETURN TO MAIN
C
30    CONTINUE
      RETURN
      END
```